Argonne Leadership Computing Facility

a preeminent resource for breakthrough science and engineering

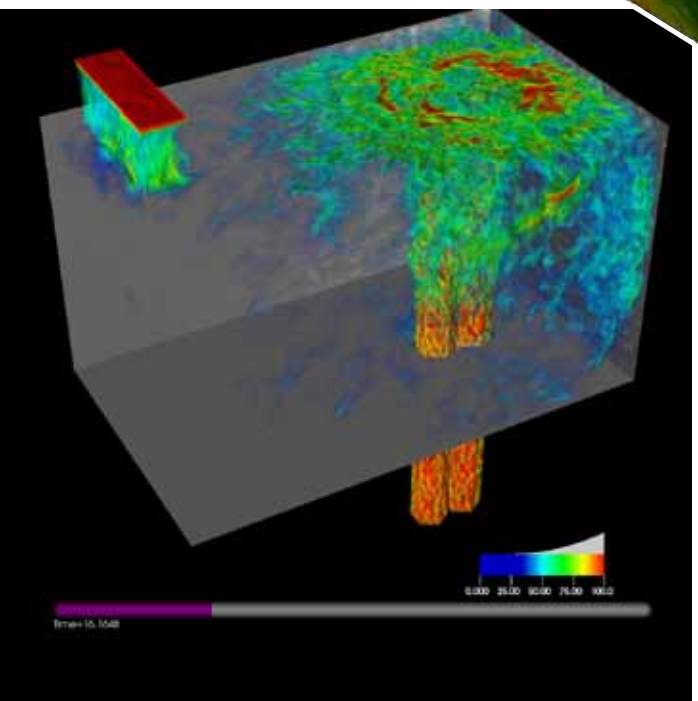
Argonne NATIONAL LABORATORY

INCITE Hours Allocated on the ALCF's Blue Gene/P: 30 Million

Making Safe, Clean Nuclear Energy Available Globally

As part of the nuclear energy program, the United States is committed to new technologies that will dramatically expand the availability of safe, clean nuclear energy to help meet the growing global energy demand. Liquid-metal-cooled fast reactors are a key component of this strategy in that they permit recycling of nuclear fuel and are expected to be economical sources of power.

Coolant-flow pressure distribution in a 217-pin wire-wrapped subassembly, computed on P=65536 processors of the Argonne Leadership Computing Facility's BG/P using Nek5000. The Reynolds number is Re~10500, based on hydraulic diameter. The mesh consists of 2.95 million spectral elements of order N=7 (~988 million gridpoints). The simulation pictured is a watershed computation, as it is the first to exceed one million elements (2.95 M used) and the first to use one billion gridpoints (0.988 B used).



This image represents the turbulent flow of coolant into a mock-up of the upper plenum of an advanced recycling nuclear reactor. The colors indicate the speed of the fluid, red representing regions of high velocity, and blue representing regions of low velocity. Coolant enters from hexagonal channels at the bottom of the plenum as two jets, each with a mean flow velocity of 1 meter-per-second, and exits from a single rectangular channel at the top. The results of these simulations will be used in conjunction with data from Argonne's MAX experimental test stand to better understand the thermal-hydraulic properties of the flow. This simulation was performed using the Nek5000 code employing 68,826 spectral elements of order N=7 and run on 8,192 core of the IBM Blue Gene/P at the Argonne Leadership Computing Facility (ALCF) at Argonne National Laboratory.

Scientific Approach

Through U.S. Department of Energy (DOE) INCITE allocations, researchers are carrying out large-scale numerical simulations of turbulent thermal transport in sodium-cooled reactor cores. These simulations will enable researchers to gain an understanding of the fundamental thermal mixing phenomena within advanced recycling reactor cores, which can lead to improved safety and economy of these pivotal designs.

Results

Argonne and University of Illinois teams are working together to validate the core hydrodynamics large-eddy simulations by comparing highly detailed simulations in similar configurations. On the Blue Gene/P at the Argonne Leadership Computing Facility, the partners are performing simulations of coolant flow in a simplified geometry that allows them to resolve all turbulent motion with no modeling assumptions. These results are being compared to the Nek5000 computations, which simulate only the largest turbulent eddies in the flow. The validated Nek5000 results are being used to benchmark steady-state Navier-Stokes codes that employ turbulence models and to provide input to reactor design codes that require only coarse (mean flow) data. Visualization support for this project is provided by the VisIt group at Lawrence Livermore National Laboratory.

INCITE Contribution

"Computations on the ALCF Blue Gene/P, made possible through a DOE INCITE award, are already yielding important results in the analysis and understanding of reactor core flows, including establishment of turbulent flow entry lengths and subassembly coolant mixing characteristics."

U.S. DEPARTMENT OF ENERGY
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LEADERSHIP COMPUTING

ALCF Contribution

"The range of scales encountered even in a single subassembly has driven the computational requirements for our Nek5000 code to unprecedented levels. The Argonne Leadership Computing Facility has proved essential for undertaking simulations at these scales."

Contact

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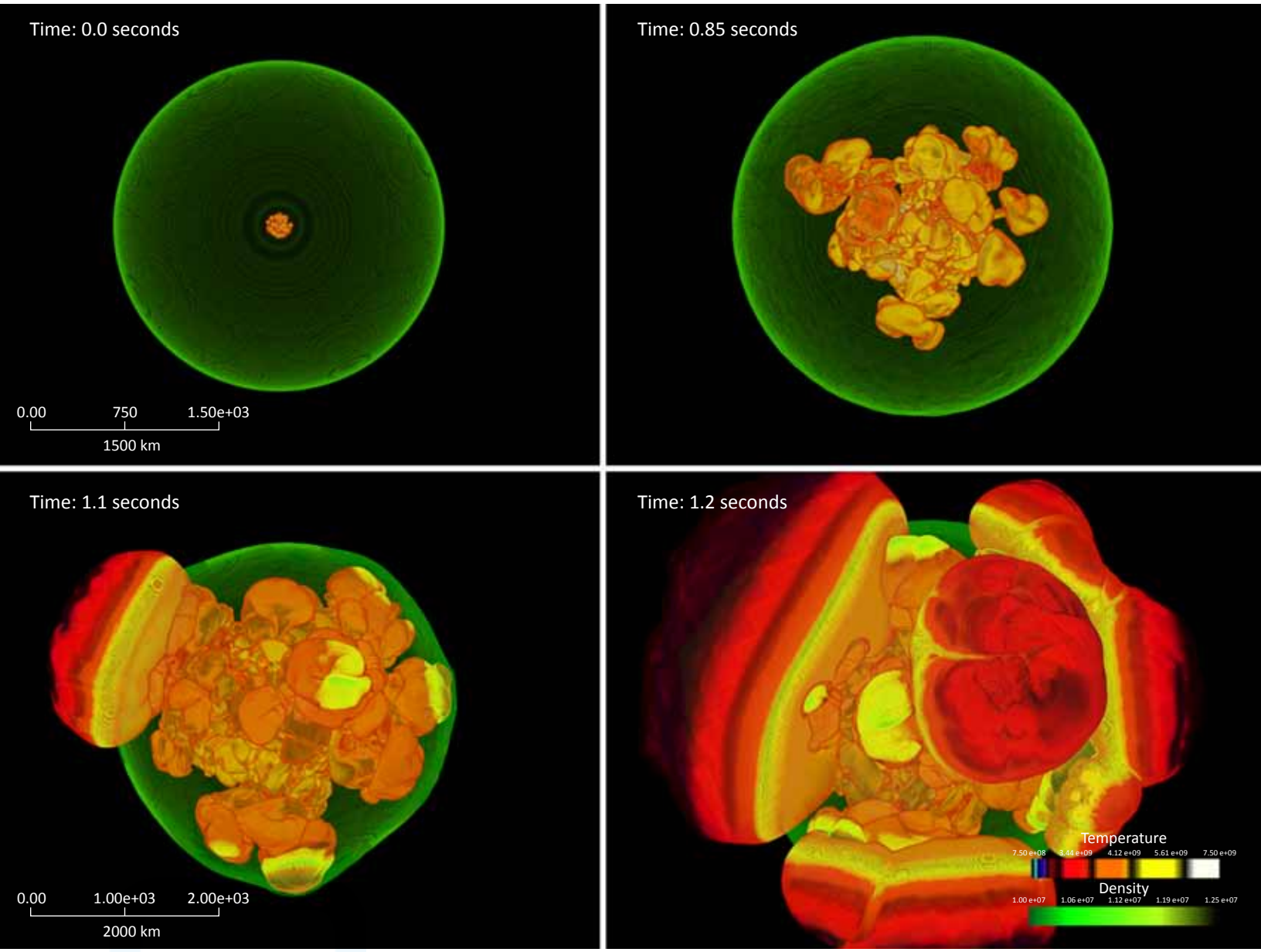
astrophysics

INCITE Hours Allocated on the ALCF's Blue Gene/P: 70 Million

How Do Standard Candles Illuminate Knowledge of the Universe?

Type Ia supernovae (SNe Ia) are among the brightest exploding stars in the universe. Observations using SNe Ia as "standard candles" led to the discovery of dark energy. Most scientists believe that using SNe Ia to determine the properties of dark energy will require a much better understanding of these explosions.



Four snapshots during a simulation of the explosion phase of the deflagration-to-detonation (DDT) model of nuclear-powered (Type Ia) supernovae. The images show extremely hot matter (ash or unburned fuel) and the surface of the star (green). Ignition of the nuclear flame was assumed to occur simultaneously at 63 points randomly distributed inside a 128-km sphere at the center of the white dwarf star. The images show volume renderings of extremely hot regions and the surface of the star [defined as the region in which the density is (1.0 - 1.25) x 10^{7} g cm^{-3}]. Upper left panel: 0.0 seconds, showing the initial distribution of ignition points. Upper right panel: 0.85 seconds, when the bubbles have become Rayleigh-Taylor unstable and developed into mushroom shapes on their way to the surface of the star. Lower left panel: 1.1 seconds, when the first plume of hot ash has made its way to the surface, and the flame front has entered the distributed burning regime, initiating a detonation. Lower right panel: 1.2 seconds, after several plumes of hot ash have reached the surface and multiple detonations have occurred, while the first detonation wave is propagating through the star. Images were created from a simulation run on the Blue Gene/P at the Argonne Leadership Computing Facility in 2009.

Scientific Approach

Researchers are using the FLASH code and time on the IBM Blue Gene/P at the Argonne Leadership Computing Facility (ALCF) awarded through the U.S. Department of Energy's INCITE program to conduct the first comprehensive, systematic validation of current models of SNe Ia and to determine the fundamental properties of buoyancy-driven turbulent nuclear combustion – a physical process that is key to SNe Ia but is not fully understood.

Results

The team has simulated all current models of Type Ia supernovae on the ALCF's Blue Gene/P. These simulations led to the discovery of robust signatures for the different SN Ia models, holding out the promise that observations can discriminate among them. The team also has simulated buoyancy-driven turbulent nuclear combustion. These simulations show that the flame surface is complex at large scales and smooth at small scales, suggesting that the burning rate may be determined by the properties of the flame at large scales.

INCITE Contribution

"The time awarded to the Center under the INCITE program has been essential to the team's ability to achieve these scientific results."

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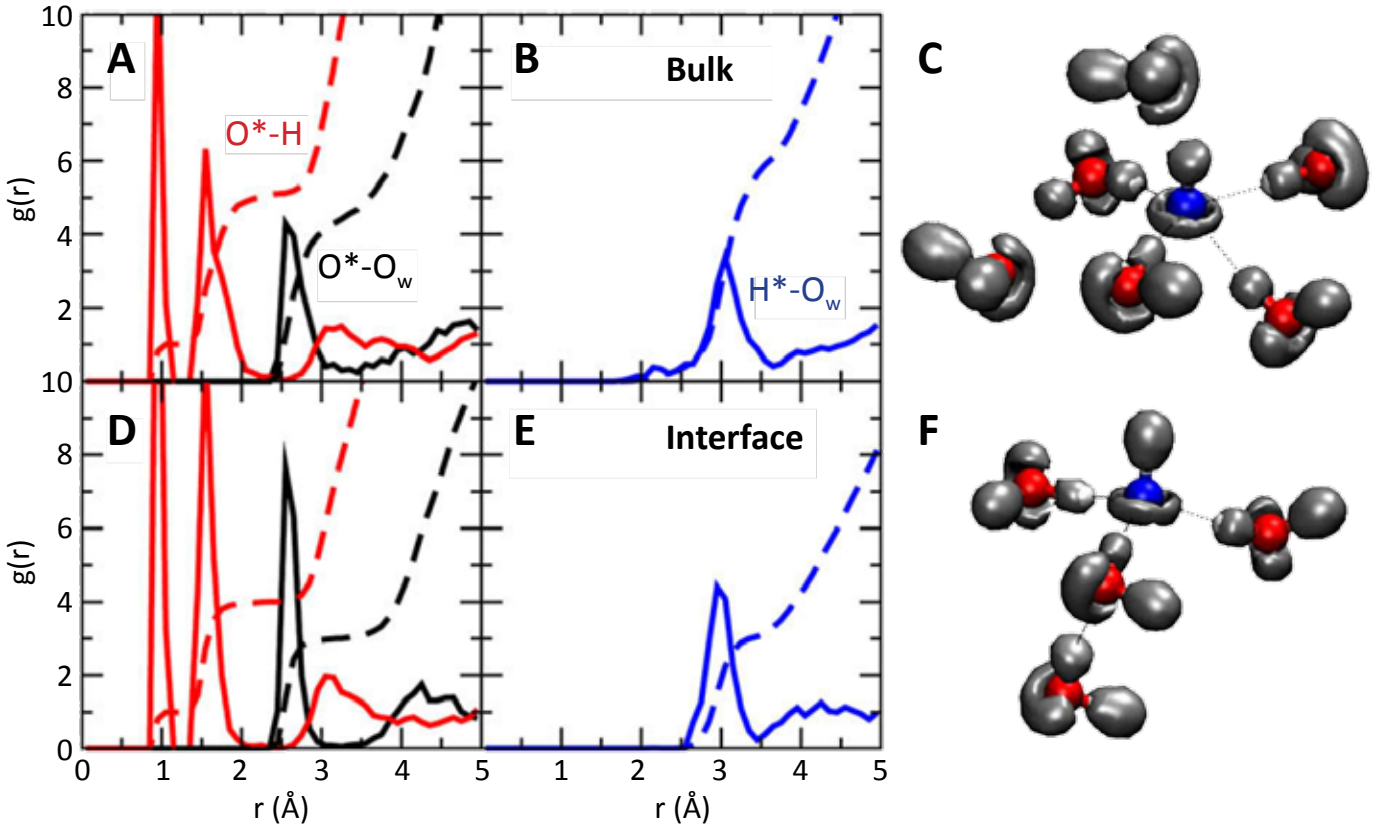
INCITE Hours Allocated on the ALCF's Blue Gene/P: 2 Million

Molecular Simulation of Complex Chemical Systems

Understanding reactions on a molecular scale is critical to solving many of the challenges facing the 21st century. However, the knowledge of reactions that lead to important phenomena in areas such as environmental science, energy technologies, and biology remains in its infancy. Leadership-class computing provides scientists with the computational molecular simulations of reactions that will lead to unprecedented discovery and will move the field of molecular simulation forward beyond incremental steps to a radically new simulation protocol.



Aqueous solvation and electronic structure of the hydroxide anion. (A) Radial distribution functions, g(r), of water oxygen (Ow) and hydrogen (H) atoms around the oxygen atom (O*) of the hydroxide anion in bulk water. (B) Radial distribution function of water oxygen atom around the hydrogen atom (H*) of the hydroxide anion in bulk water. (C) Electron localization functions [52] (gray surfaces) depicting the location of the valence electrons of the hydroxide anion (blue) and water molecules (red) in its solvation shell in bulk water. (D)–(F) same as (A)–(C), but for the ion at the interface. In panels (A, B) and (D, E), the dashed lines depict the running coordination numbers derived from the corresponding radial distribution functions.

Scientific Approach

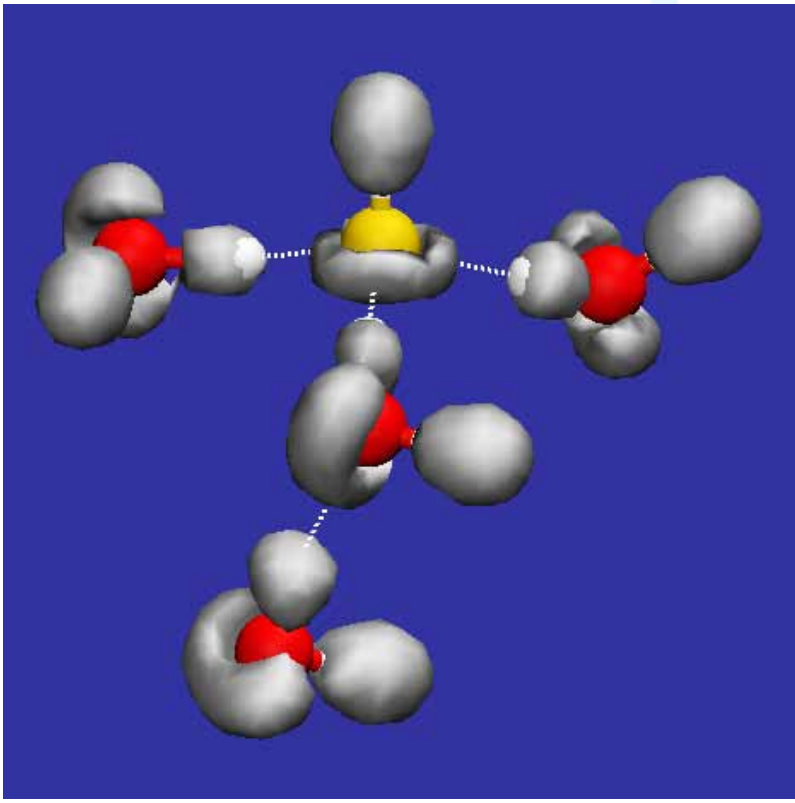
Researchers at Pacific Northwest National Laboratory and their collaborators (New York University, University of California, Irvine, and Lawrence Livermore National Laboratory) are using their INCITE allocation to apply statistical mechanical sampling methods in conjunction with Density Functional Theory (DFT)-based interaction potentials to make detailed models of chemical processes at interfaces. They are conducting their research on the Blue Gene/P supercomputer at the Argonne Leadership Computing Facility (ALCF). The basic chemical physics of these leadership calculations will provide a detailed, molecular-scale picture of ions and reactions near interfaces.

Results

The findings on the OH- have provided a picture where there is a weak propensity for the anion at the air-water interface, a prediction that is exactly opposite of that deduced from classical empirical potentials. The reason for this can be found in the hydroxide anion's unique electronic structure. The change in structural moieties facilitated by the unique electronic structure of the anion promotes its presence at the air-water interface with little free energy penalty. These important findings have reinforced the notion that novel chemistry can occur in the vicinity of the air-water interface, and the necessity of Leadership Class Computing through our INCITE 2008-2009 to help understand it. Chem. Phys. Lett. 481, 2-8 (2009).

Future Efforts

Future efforts will probe other important ions, namely H_3O^+ with results on OH^-, and will allow researchers to determine the differences in the pH of interfaces and bulk. This fundamental result will have far-reaching implications for the basic understanding of chemical processes at interfaces.



A figure illustrating the peculiar electronic structure and three-fold coordination of the hydroxide anion (OH-) depicted in yellow surrounded by neighboring water molecules (depicted in red) in a configuration extracted from the vicinity of the air-water interface.

INCITE Contribution

"The use of leadership-computing resources, in conjunction with fast electronic structure algorithms, has been critical to the correct statistical mechanical sampling on the systems of adequate spatial dimensions. INCITE resources are enabling researchers to take quantity (system size and number of CPUs) to a new quality (elucidation of chemical process in heterogeneous environments). These unique calculations contribute directly to DOE's Molecular Theory and Modeling program funded by the Basic Energy Sciences, Chemical Sciences, Geosciences and Biosciences Division."

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

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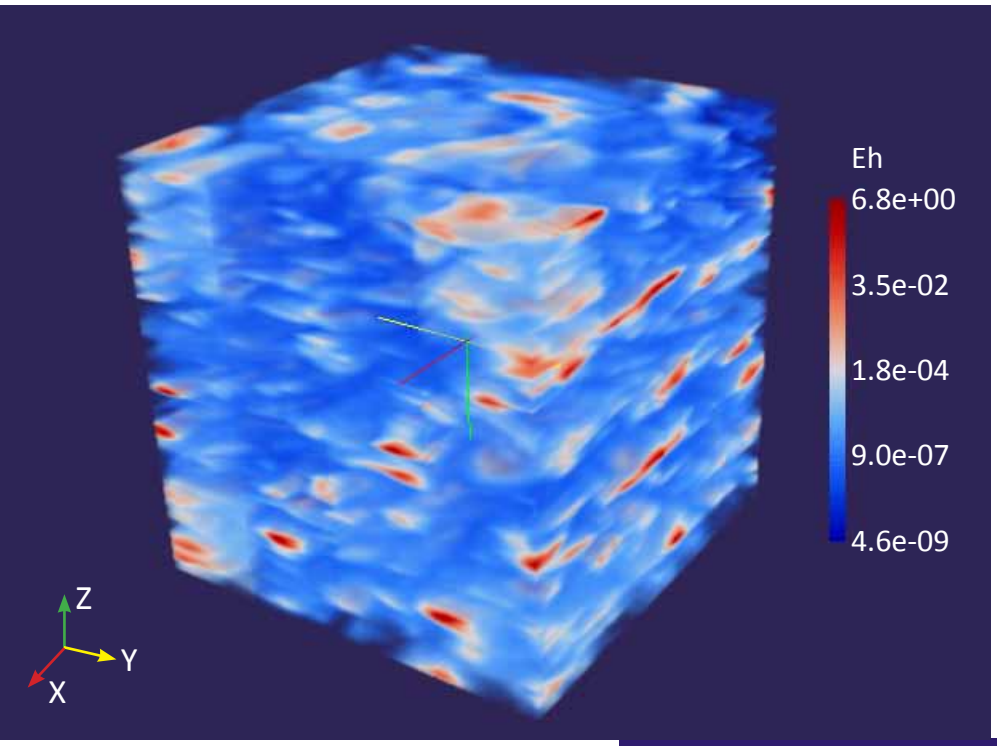
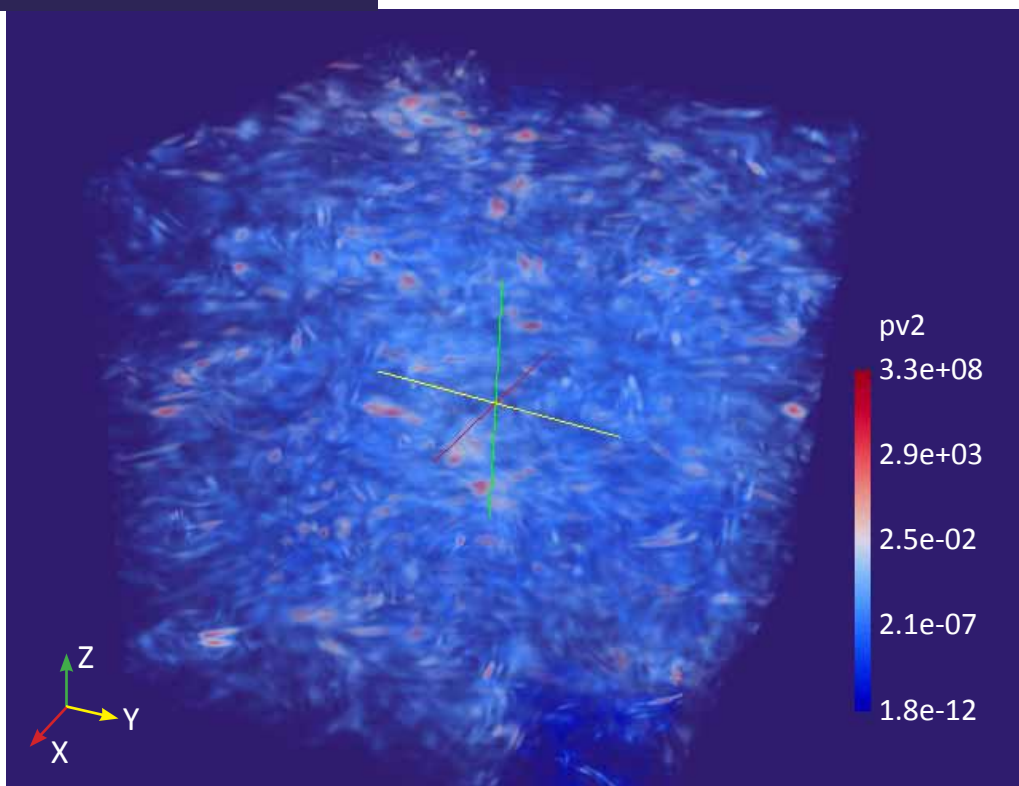
INCITE Hours Allocated on the ALCF's Blue Gene/P: 25 Million

Numerical Study of Multiscale Coupling in Low-Aspect Ratio Rotating Stratified Turbulence

The information scientists glean from representative models is only as accurate as the models themselves. Current climate models make use of approximations that are accurate over a large part of the ocean, but do not provide the high resolution necessary for accuracy at a regional level (e.g., the Gulf of Mexico or the Arctic basin).



For this flow, in which the stratification is stronger than the rotation, the energy is seen to be organized into coherent flattened structures in a layering of the flow.



For the same flow, a different but equally important quantity called the potential enstrophy does not show any indication of organizing into two-dimensional structures, but rather remains three-dimensional at all scales in the flow.

Scientific Approach

A research team comprised of Susan Kurien (Los Alamos National Laboratory), Leslie Smith (University of Wisconsin, Madison), Mark Taylor (Sandia National Laboratories) and Ramesh Balakrishnan (Argonne National Laboratory) are performing extremely high-resolution simulations to quantify the behavior of rotating and stratified turbulent flows in which multiple time and spatial scales may be simultaneously important, and for which non-hydrostatic effects are not negligible and a statistical description becomes necessary. The simulations are being conducted on the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF). This work may result in critical adjustments of the fluid dynamics component in models—especially in those models used for prediction of long-term phenomena like climate change, and may lay the groundwork for next-generation climate research.

Results

Researchers have computed, analyzed, and visualized rotating and stratified turbulence for various aspect ratio domains. Their high-resolution simulations have allowed them to verify theoretical predictions about energy and potential enstrophy distribution in the small scales. In the particular case of stratification-dominated turbulence, the accompanying figures show how the horizontal energy is organized into flat disk-like structures, while the potential enstrophy in the same flow continues to exhibit largely 3-dimensional structure in the small scales.

Future Efforts

Continued efforts aim to achieve even smaller aspect-ratio domains with rotation and stratification parameters closer to those expected in the ocean and atmosphere. Such simulations run for very long times will tell researchers how the small-scale turbulence affects the climate scales in both space and time.

INCITE Contribution

"The resolutions and parameter regimes of interest in our research would be impossible to achieve without the exceptional caliber of resources made available by the INCITE program."

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

ALCF Contribution

"The prompt and professional support of ALCF staff has enabled us to get initial results and make significant progress in a remarkably short period of time."

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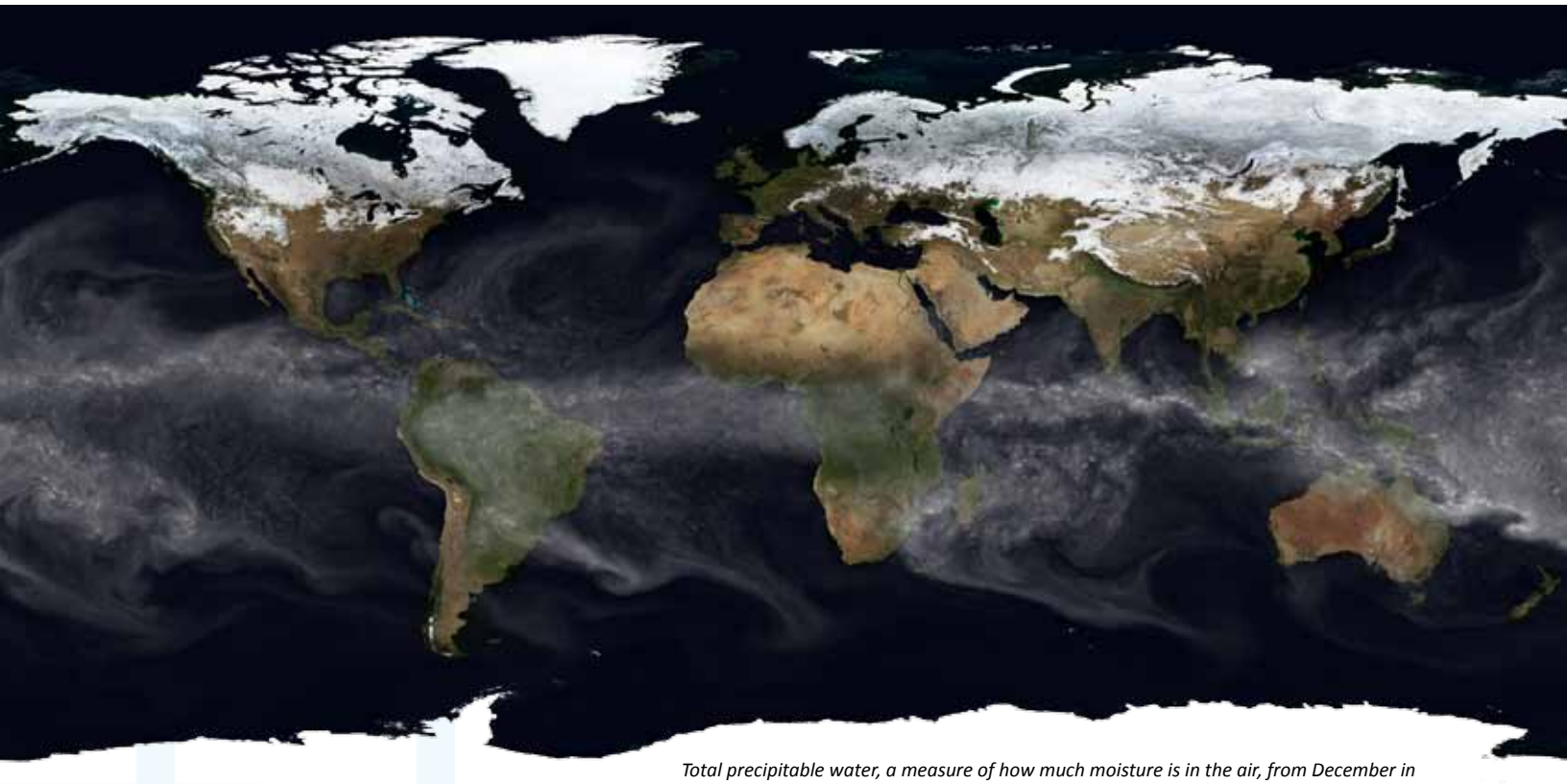
INCITE Hours Allocated on the ALCF's Blue Gene/P: 7.5 Million

How Can More Intricate Climate Models Help Curb Global Warming?

Global warming occurs due to the massive amounts of carbon dioxide and other greenhouse gases released into the Earth's atmosphere from human activity. Scientists are alarmed at the rate at which global temperatures are rising—far faster than previous aggressive estimates. Global warming is consistent with events already observed such as intensified tropical storms and the decrease in Arctic sea ice cover. All of the climate models currently in use predict further global average warming if greenhouse gas release continues.

Scientists are now concerned with the regional affects of global warming where models have less agreement. Some regions will see warming far above the global average. Other regional phenomena such as floods, heat waves, droughts, and severe weather are expected to change under a warmed climate. An important element in predicting these changes is to increase the resolution of climate models.

Advanced computation, like that possible on the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF), allows researchers at the National Center for Atmospheric Research (NCAR) and their partners at U.S. Department of Energy (DOE) labs to develop more complex and intricate climate models. The vital information these improved models provide will help guide policy so scientists can take steps to curb global warming and prevent further disruption to the planet's climate.



*Total precipitable water, a measure of how much moisture is in the air, from December in a global simulation of the atmosphere at 1/8th of a degree. (*Image credit: Jamison Daniel, ORNL National Center for Computational Sciences)

Scientific Approach

DOE awards individual allocations of computing resources for climate studies across multiple laboratories through the INCITE program. In turn, the Climate Computational End Station (CCES) organizes and coordinates these computational efforts.

Using ALCF resources, CCES is advancing climate science through both an aggressive model development activity and an extensive suite of climate simulations—particularly the correct simulation of the global carbon cycle and its feedbacks to the climate system, including its variability and modulation by ocean and land ecosystems.

Results

Researchers at NCAR and Sandia National Laboratory have used their ALCF allocation to test a new, highly scalable method for solving the fluid dynamics of the atmosphere. This model, called HOMME, has been shown to run with resolution as high as 1/8th of a degree of latitude on over 80,000 cores.

Future Efforts

Next year, researchers will use HOMME to perform standard climate model benchmark simulations for comparisons with other models. The team will also test the new version of the Community Climate System Model (CCSM) on the ALCF's Blue Gene.

INCITE Contribution

"The INCITE-supported development of a massively parallel CCSM is absolutely critical for climate scientists who will be carrying out the massive set of societally and policy relevant simulations for the IPCC AR5. These simulations will require much higher model resolutions, using much more expensive biogeochemistry and atmospheric chemistry packages, which must run efficiently at scale on the next generation of massively parallel machines."

ALCF Contribution

"Without access to the resources at the ALCF, we would not have had the large number of processors necessary for testing our advanced models."

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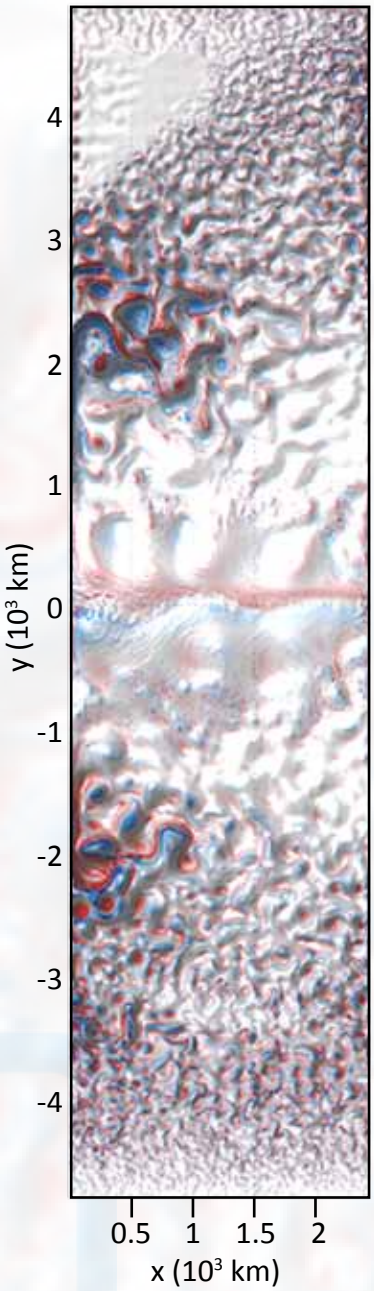
INCITE Hours Allocated on the ALCF's Blue Gene/P: 5 Million

What Role Do Eddies Play in Meridional Overturning Circulation?

Unlike the atmosphere, which is heated "internally" by radiative processes, the ocean is differentially heated only at the top. A fundamental question in physical oceanography is how the thermal (and haline) gradients are transferred from the ocean surface to the abyss. The processes that maintain the oceanic deep thermocline and the abyssal stratification are not understood, making accurate prediction of future climate scenarios impossible.



The figure shows a snapshot relative vorticity (in colors) and pressure (relief) at 100 m depth in a simulation with realistic, though idealized, forcing. Note the abundance of eddies away from the equator (at y = 0) and the large-scale separation between the smallest energetic features and the simulation domain. The color range spans ±5e-4 $s^{(-1)}$. The domain is a simple "notched box" ocean with vertical walls and a periodic channel in the southernmost 1200 km.

Scientific Approach

Using the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF), researchers analyzed high-resolution models of the ocean component of the climate system in domains of moderate size that include external parameters such as wind speed, surface temperature, and abyssal mixing.

Results

Significant findings include the following: 1) Eddies are essential to balance the creation of available potential energy by the large-scale flow; 2) Deep stratification and the overturning circulation are strongly controlled by the dynamics in a zonally reentrant southern channel (analogous to the Antarctic Circumpolar Current in the Southern Ocean); 3) The effects of a thin coastal upwelling region can be represented by a set of effective boundary conditions that relate the longshore buoyancy gradient to eddy fluxes of buoyancy and potential vorticity away from the boundary. Therefore, it is not necessary to resolve these regions in ocean models if the effective boundary conditions are used.

Future Efforts

The near-term focus will be to generalize the effective boundary conditions to regions with strong diabatic forcing and implement these generalized boundary conditions in a coarse-resolution model, verified through a series of high-resolution simulations.

INCITE Contribution

"Allocations on INCITE computers have allowed us to complete over 3,000 years of simulations spanning more than 17 different variations in geometry, surface forcing, and diffusivity."

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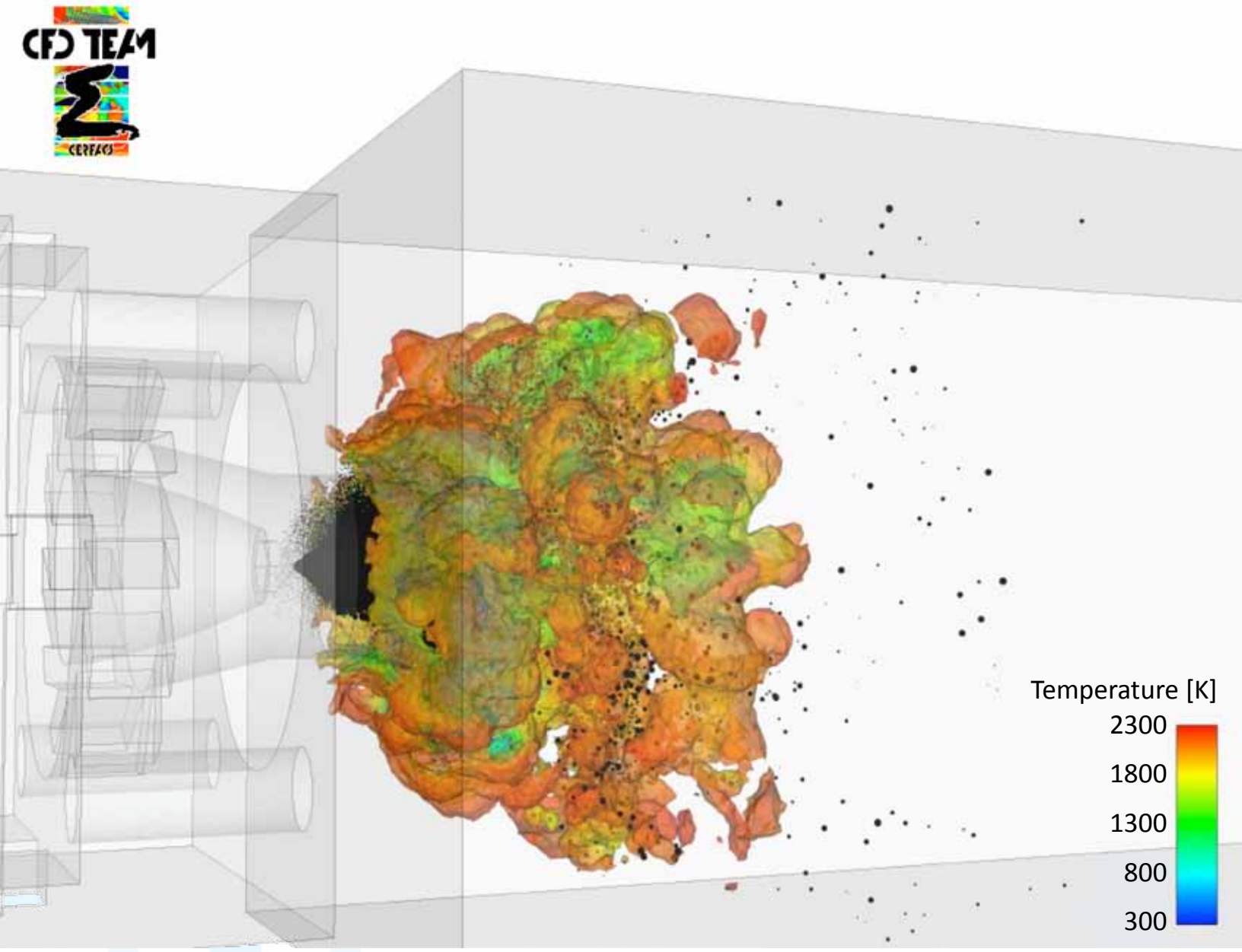
INCITE Hours Allocated on the ALCF's Blue Gene/P: 8 Million

What Does Massively Parallel Simulation of Combustion in Gas Turbines Reveal?

Among all Computational Fluid Dynamics (CFD) methods, Large Eddy Simulation (LES) techniques offer the ability to predict instantaneous flow characteristics by resolving the spatial and temporal evolution of turbulent flow structures. LES techniques also provide significantly more accurate results for flows involving flow separation or flame/acoustic interactions.



Large-Eddy Simulation of the reactive two-phase flow simulation inside an experimentally investigated aeronautical combustor using an Euler-Lagrange formalism. The flame is evidenced through an iso-reaction rate colored by temperature. Particles are shown as black spheres, which scale with particle diameter.

Scientific Approach

Researchers at the European Center for Research and Advanced Training in Scientific Computation (CERFACS) are developing and applying the LES CFD approach for the simulation of unsteady reacting flows. They are focusing on technically challenging issues in real gas turbines, thereby demonstrating the usefulness of LES in the design process. These issues, which are beyond the capacities of currently used CFD tools, include ignition, re-ignition, flame quenching, and instabilities.

While CFD research is often limited to a single burner, combining LES and the massively parallel computer resources at the Argonne Leadership Computing Facility (ALCF) allows CERFACS researchers to investigate the interaction of multiple burners in annular chambers to study important physical mechanisms such as burner interactions, azimuthal acoustic modes generation, flame propagation from one burner to its neighbors, or how quenching occurs.

Data gathered from this research will have real-world application in energy production (e.g., industrial gas turbines) and propulsion (e.g., helicopter and aircraft engines).

Results

Researchers have reproduced the behavior of a gas turbine demonstrator equipped with 15 burners and a new injector design. The LES singled out the presence of a thermo-acoustic instability that impacts the flow behavior. However, these results reveal that, in this case, flame anchoring is not jeopardized by the instability. This fact was also observed in laboratory tests and confirmed that LES can be used to discriminate designs.

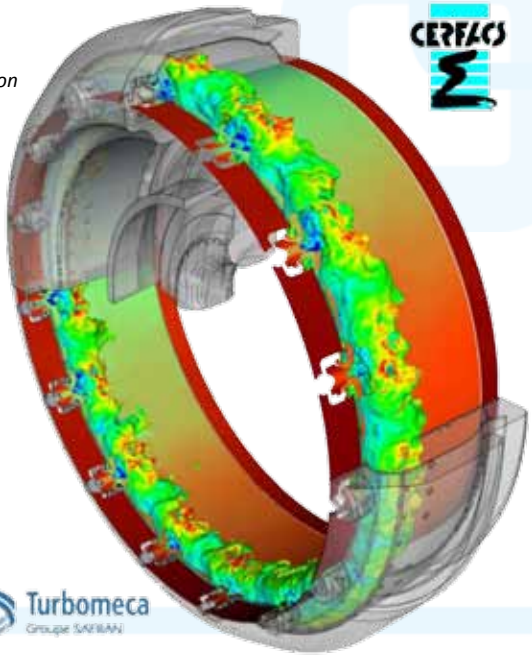
At the same time, the first studies taking into account the presence of a liquid phase in laboratory test cases were undertaken and yielded promising results.

Future Efforts

Integrating the liquid fuel injection in the gas turbine demonstrator is the next logical step. This will allow researchers to study the impact of the liquid evaporation on the flame structure as well as the possible emergence of thermo-acoustic instabilities due to evaporation delays. Performing this full chamber LES will be much more challenging than LES performed up to now. It will involve both top-of-the-edge modeling (e.g., for spray), as well as innovative computer science techniques (dynamic load balancing and conditional domain decomposition).

INCITE Contribution

"The simulations performed to date would have taken over a year to perform on our current accessible computers. Also, parametric studies are impractical because having four or more simulations running for a year is not possible. Access to INCITE computers has allowed both. We have been able to demonstrate the important aspects of combustion instabilities, ascertain predictions, and confirm what we found via experiments. This validates the whole computational approach applied in our preliminary full gas turbine simulations."



Pressure fluctuation (cylinder) and temperature iso-surface on a helicopter chamber demonstrator.

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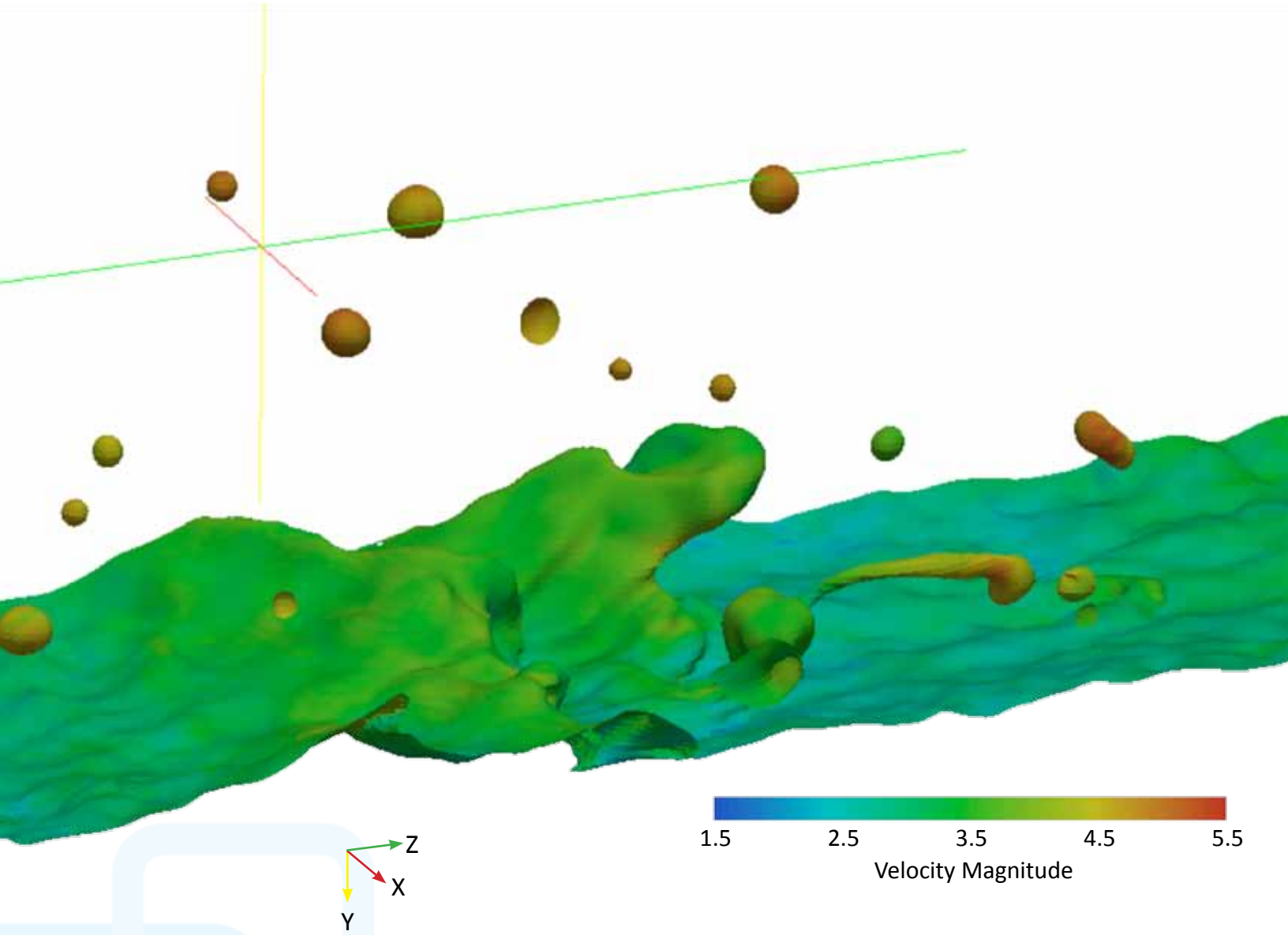
INCITE Hours Allocated on the ALCF's Blue Gene/P: 5 Million

Petascale Adaptive CFD for Anisotropic Flows

Numerical methods for partial differential equations have reached a level of maturity for a range of physical problems, including fluid mechanics, solid mechanics, electromagnetics, biomechanics, and others. But such problems are prohibitively expensive to consider with methods using structured grids (mesh grows too large), explicit techniques (time step becomes too small), and/or procedures with limited scalability (time-to-solution takes too long). Unstructured and implicit techniques may be employed but must be scalable to solve extremely large practical problems and yield dramatic compression in time-to-solution(s) for a fixed-size problem.



Annular flow: liquid-vapor interface colored by local flow speed. High-speed vapor core drives vapor film to develop waves that break to produce drops and bubbles.

Scientific Approach

Researchers have developed a parallelization paradigm and associated procedures that enable their implicit, unstructured mesh flow solver to achieve strong scalability on leadership-class computers. The techniques are amenable to other linear or nonlinear, explicit or implicit numerical methods for partial differential equations. Complex flow problems are efficiently addressed by adapting the grid to match the solution's highly anisotropic flow features.

Results

In an abdominal aortic aneurysm model with O(10^8) elements, researchers achieved near-perfect strong scaling from 512 cores up to 16,384 cores of the Blue Gene/P Intrepid at the Argonne Leadership Computing Facility (ALCF).

On a mesh with O(10^9) elements, researchers performed strong scaling studies on Intrepid and observed a near-perfect strong scaling (93% or above) for the equation-formation stage all the way to the full system scale.

These results demonstrate the ability of the current procedures to achieve strong scalability on prospective supercomputers with hundreds of thousands of cores.

Future Efforts

These techniques will be advanced and employed to understand complex flow physics, yielding insight into open scientific questions such as active flow control on 3-D wind turbine configurations and multi-phase flows like those occurring in accident conditions (e.g., burnout) in heat exchanger tubes or core breach in Generation IV reactors.

INCITE Contribution

"The strong scalability of Intrepid allows 1 billion element discretizations of the transient Navier-Stokes equations to be solved in just over one second per time step. This dramatic compression of time makes extremely large simulations relevant to time critical analysis."

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

ALCF Contribution

"ALCF computing resources enabled taking the PHASTA code to unprecedented scale – 40× the processor count of other resources available to the project."

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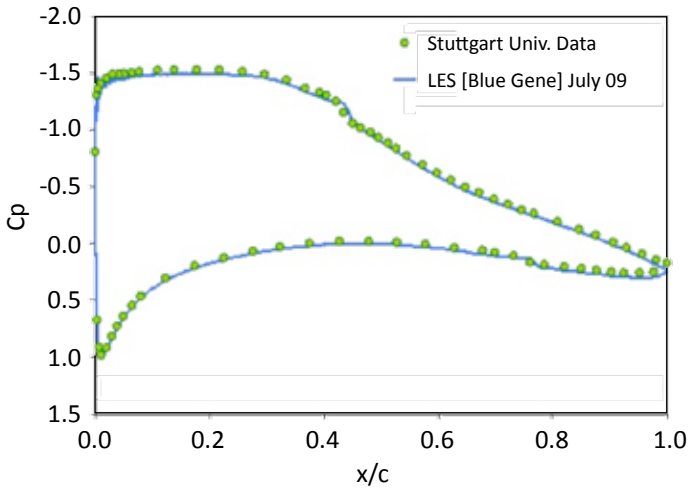
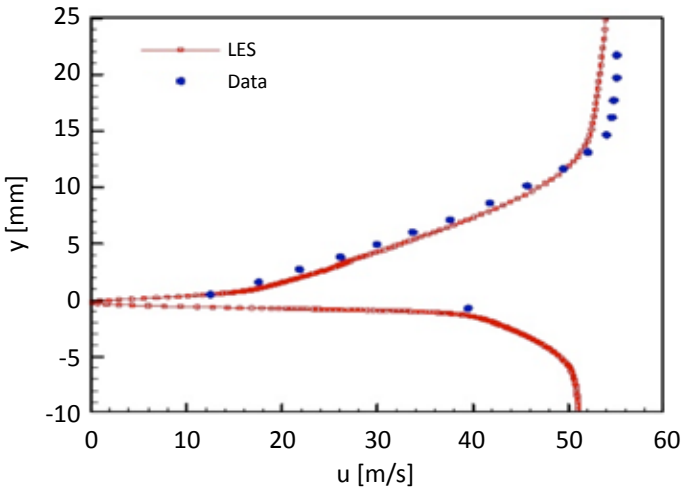
Large-Eddy Simulations Enable GE Research on Quiet Wind Turbines

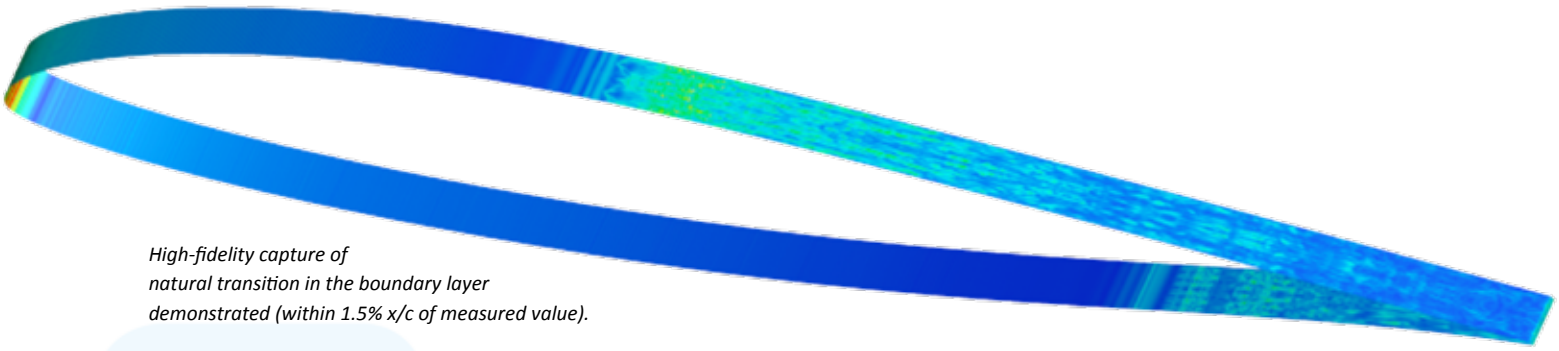
Reducing aerodynamic noise is critical to the viability of next-generation "green" low-carbon/GHG emission energy systems e.g., wind turbines. Scientists at GE Global Research (GEGR) are investigating methods to reduce airfoil trailing edge noise—a key component in wind turbine noise generation. Predicting noise directly from first principles, while numerically expensive, is a promising method to characterize noise for hard-to-measure details and sources.



Computed pressure matches wind tunnel measurements.



Computed mean u (streamwise) velocity in excellent agreement with measured wake data just off the trailing edge.



High-fidelity capture of natural transition in the boundary layer demonstrated (within 1.5% x/c of measured value).

Scientific Approach

Compressible Large Eddy Simulation (LES) methods have been used to simulate a wind turbine airfoil (DU-96) operating at a realistic Reynolds number (2.5×10^6). The consequent resolution needed to model the natural transitional flow and the sensitive acoustics results in a mesh with 240 million points, covering a 4.5 % span extent. The calculation was done with 8,192 cores on the IBM Blue Gene/P at the Argonne Leadership Computing Facility (ALCF) after 2008 successes in porting/demonstrating scalability at Argonne National Laboratory.

Results

Comparisons with available experimental data, especially flow, show that the LES predictions are successful in predicting key flow phenomena, viz., the transition location, wake profiles at the trailing edge of the airfoil, and pressure distribution. Refinements to the higher-order flow solver and meshing best practices were needed to obtain accurate results of the wall-shear evolution as the flow transitions from laminar to fully turbulent flows. Acoustic calculations are in progress.

Future Efforts

With the first proof-of-concept aero and acoustic LES calculation completed, the team will pursue the use of LES+HPC to a) develop noise source models for use in lower-order tools and b) improve the efficiency/accuracy of the LES methodology – both algorithmically and from a parallel scalability beyond 8K cores.

ALCF Contribution

"Simulation-based aeroacoustics via large-scale computing – the focus of this collaboration with ALCF – is a key enabler to tackling the yield-limiting noise barrier for wind turbines. The Discretionary Allocation on Blue Gene/P has enabled GE to use Large Eddy Simulations to understand the physics of noise generation in boundary-layers and wakes at realistic conditions; as this technology develops, it will accelerate GE's ability to design quieter and larger blades and significantly increase the energy yields possible from the wind portion of the world's renewable portfolio."

--Dr. Gary Leonard
Global Technology Leader
Energy and Propulsion Technologies
GE Global Research

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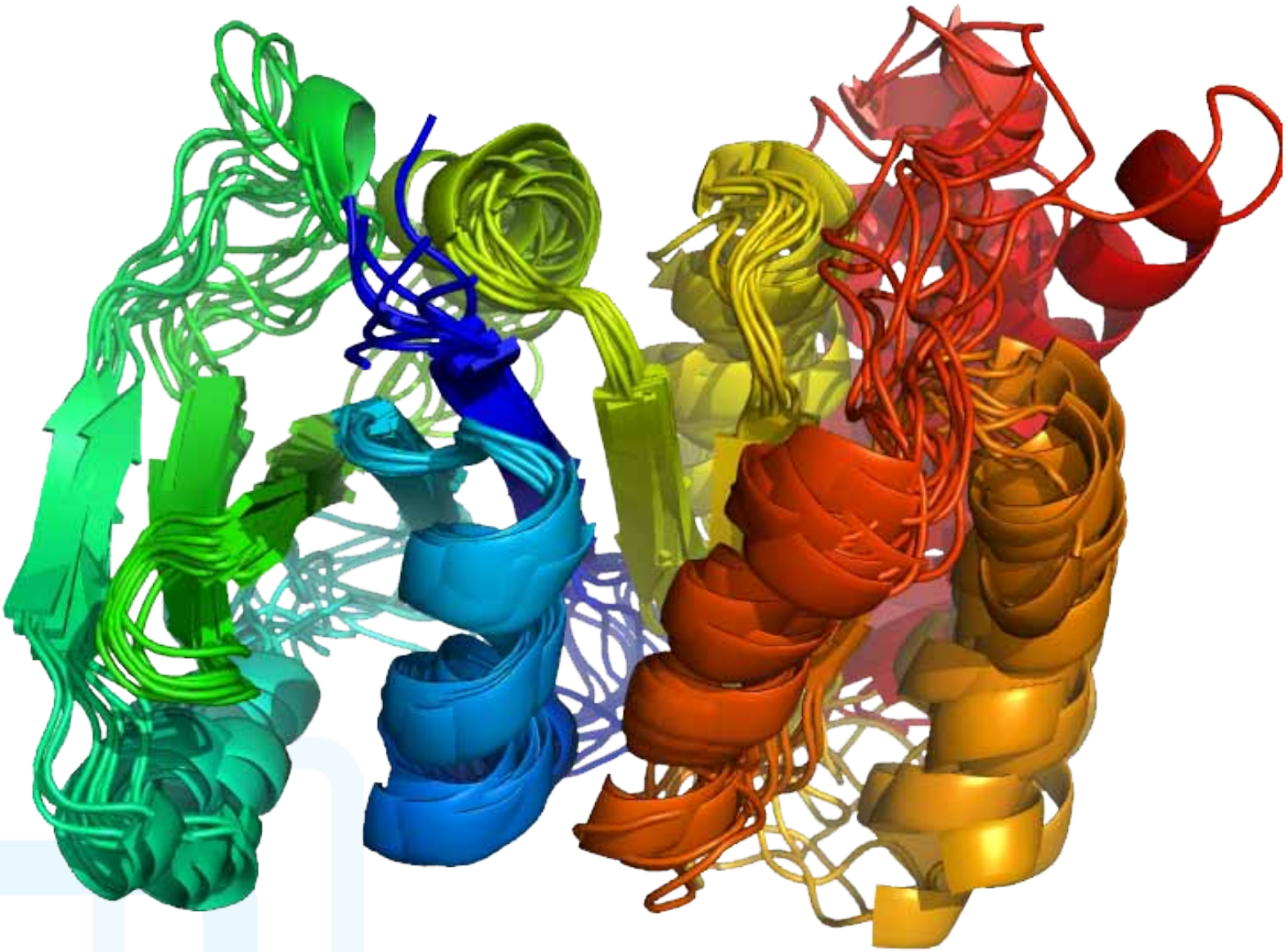
INCITE Hours Allocated on the ALCF's Blue Gene/P: 12 Million

How Do Researchers Predict the Structures of Biologically Important Proteins?

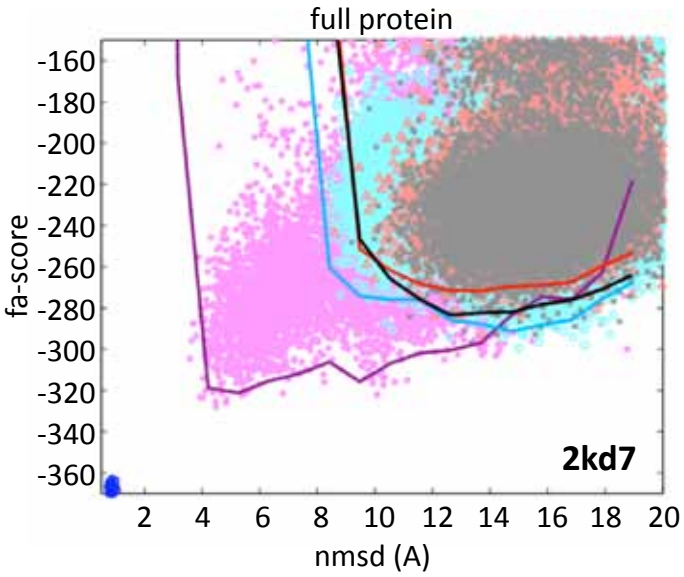
Proteins are the workhorse molecules of all biological systems. A deep and predictive understanding of life thus requires a detailed picture of their structure. Conventional protein structure determination using nuclear magnetic resonance (NMR) relies primarily on side-chain proton-proton distances. The necessary side-chain chemical shift assignment, however, is expensive and time-consuming, with possibilities for error. Moreover, approaches to NMR structure determination for larger proteins usually rely on extensive deuteration, which results in losing much of the proton-proton distance information. Sparse structural data can be obtained from backbone-only experiments like orientational restraints from residual dipolar couplings and amid proton distances from NOESY spectra. These experiments are readily applicable even to fully deuterated and large proteins.



Researchers determined this large protein, ALG13, which is 200 amino acids in length, with a new methodology called "NMR structure determination without side-chain assignments."

Scientific Approach

To determine NMR structures without side-chain chemical shift information, researchers incorporate backbone chemical shifts, residual dipolar couplings, and amide proton distances into the Rosetta high-resolution modeling methodology. To exploit the weak guidance signal provided by the sparse constraints, they developed an iterative scheme similar to a genetic optimization algorithm. A pool of the fittest individuals (e.g., lowest energy conformations) is maintained, and its worst part is replaced with offspring. The breeding or crossover of highly fit species (e.g., low energy conformations) is implemented as a Monte Carlo optimization that recombines features of previously found low-energy conformations. The type of features selected for recombination is adapted to the resolution of the pooled low-energy structures.



Comparison of different optimization methods for protein 2kd7. Purple and cyan, genetic algorithm. Red and black, conventional Rosetta optimization. Purple and red, use of residual dipolar couplings and amide proton distances as sparse constraints.

Results

The iterative protocol increased the size range of accessible protein structures compared to the conventional Rosetta protocol. Researchers consistently solve protein structures up to 200 residues. Currently, they are determining the size range of this method and are testing further improvements. The INCITE program has been and will continue to be invaluable in its development.

Future Efforts

Our INCITE work is focused on three areas currently. The first area is computing protein structures from very limited experimental data. With the INCITE computing resources, we are optimistic about developing methods which allow determination of the structures of proteins over 200 amino acids by NMR, which would be a big breakthrough in this area. The second area is designing proteins to bind very tightly to specific regions on a specified target. Over the next 6-12 months we will be using INCITE to design many proteins predicted to bind with high affinity to and neutralize the virus; these designs will be then tested experimentally, first for binding to the virus and then for neutralization. We will also be developing binders to other pathogens. The third area is design of new enzyme catalysts. In the next year, we will use the INCITE resources to design catalysts for hydrogen production, solar capture, and other energy-related applications.

INCITE Contribution

"The INCITE program has been absolutely indispensable for our research. Our work on computing protein structures and designing new protein inhibitors simply would not be possible without it."

ALCF Contribution

"The ALCF staff have been amazingly helpful in making available the computing resources we have needed and in helping us to best take advantage of them. The guidance they have provided, and their willingness to work with us to provide the resources we need when we have needed them have been absolutely terrific."

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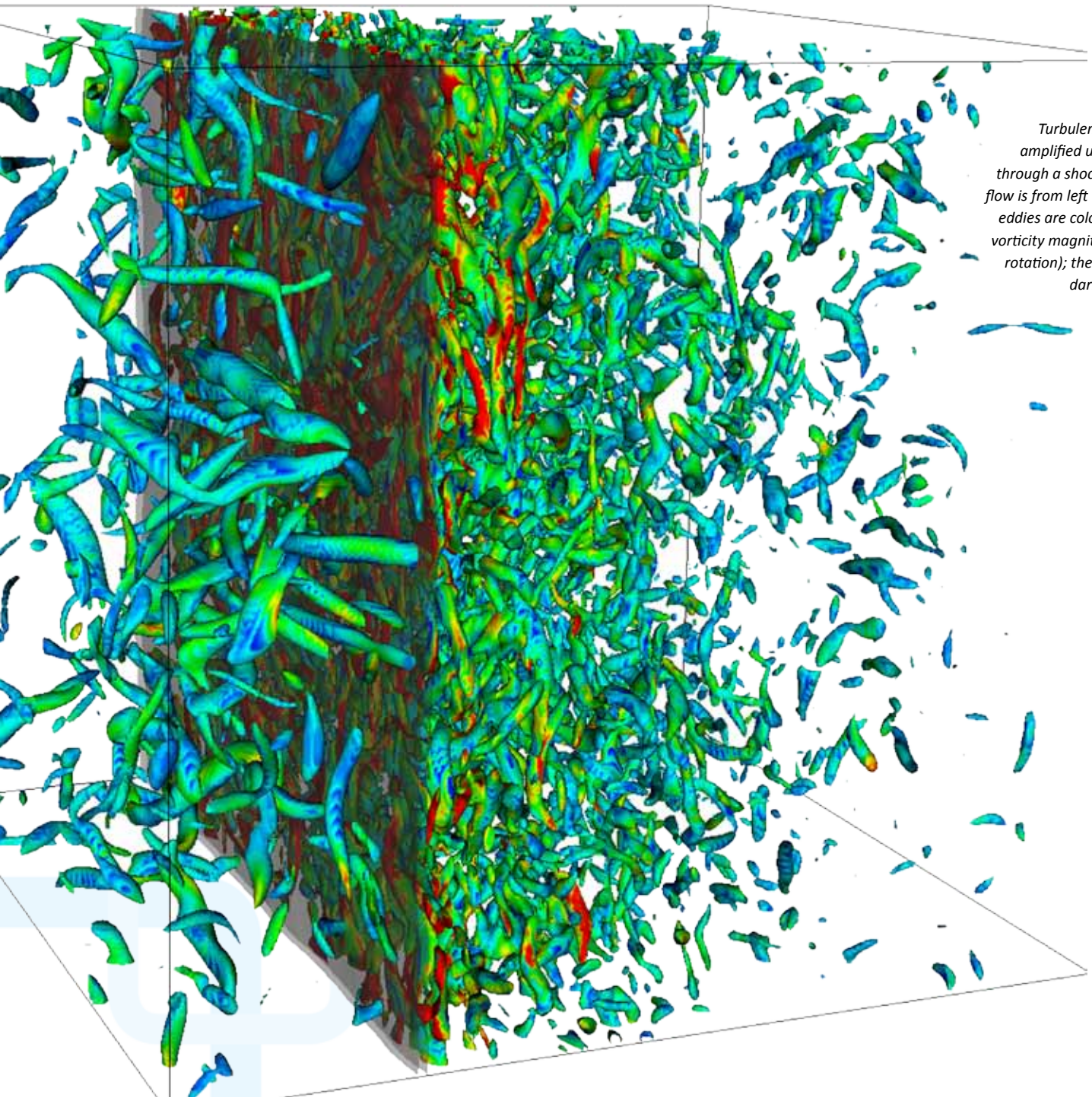
INCITE Hours Allocated on the ALCF's Blue Gene/P: 8 Million

Fundamental Study of Shock/Turbulence Interaction

Interactions between shock waves and turbulence adversely affect the stability of the flow through supersonic propulsion systems. Inadequate models—due to a poor understanding of the shock/turbulence interaction phenomenon—result in designs that sacrifice performance for stable operation. A better understanding of the fundamental physics would lead to more accurate turbulence models for improved efficiency in supersonic aircraft design.



Turbulent eddies are amplified upon passing through a shock wave. The flow is from left to right. The eddies are colored by their vorticity magnitude (rate of rotation); the shock is the dark thin sheet.

Scientific Approach

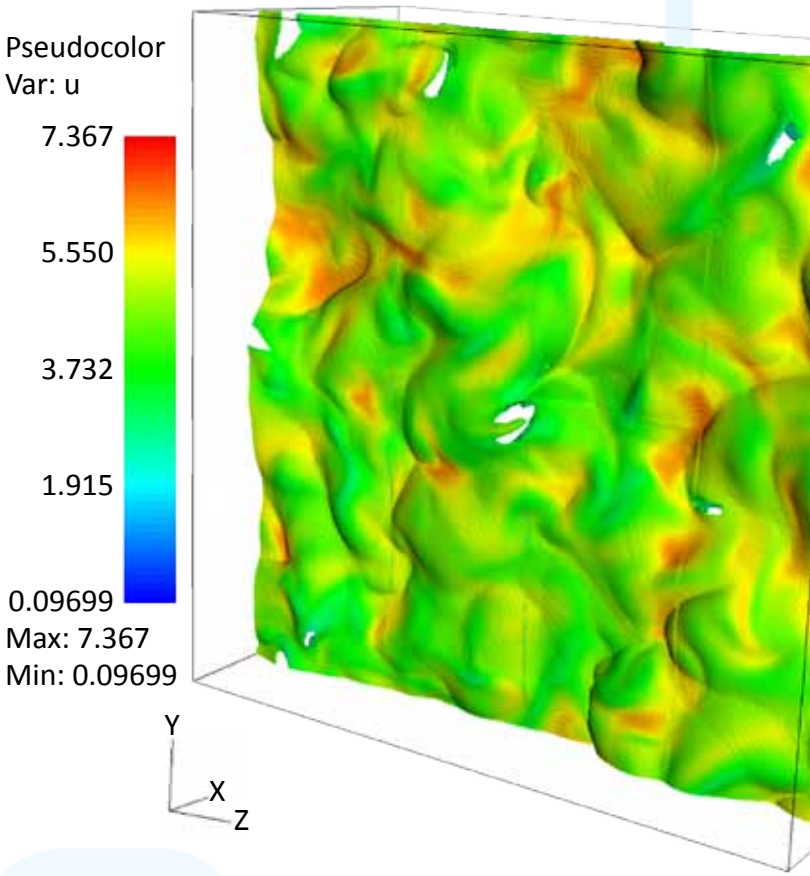
The Blue Gene/P at the Argonne Leadership Computing Facility (ALCF) is computing a set of canonical shock/turbulence interactions at unprecedented fidelity with sufficient grid resolution to accurately capture the smallest turbulent eddies. The datasets are then analyzed to elucidate how the turbulence is affected by the shock wave, and vice versa.

Results

The simulations show that the post-shock turbulence rapidly becomes isotropic at the smallest scales, but that the largest eddies remain anisotropic for a long distance. This result contradicts linear theory and shows that nonlinear effects are important in the post-shock evolution of the turbulence. In contrast, the amplification of turbulence kinetic energy during the interaction is in very close agreement with linear theory. Furthermore, results show that the instantaneous shape of the shockwave is highly distorted for strong incoming turbulence, and that the turbulence can even "punch holes" in the shock where the compression is entirely smooth.

Future Efforts

The next challenges are to develop robust, accurate engineering turbulence models and to further elucidate how the instantaneous eddies evolve through, and immediately behind, the shockwave.



Strong incoming turbulence is capable of significantly distorting the nominally normal and flat shock wave, and even to "punch holes" through it.

INCITE Contribution

"These computations are tremendously costly, requiring 4,096—16,384 cores, with each run generating hundreds of gigabytes of data. This study would not be possible without the level of computing provided by the Department of Energy's INCITE program."

ALCF Contribution

"Computer scientists from ALCF were instrumental in the initial porting of the code to the Blue Gene/P machine."

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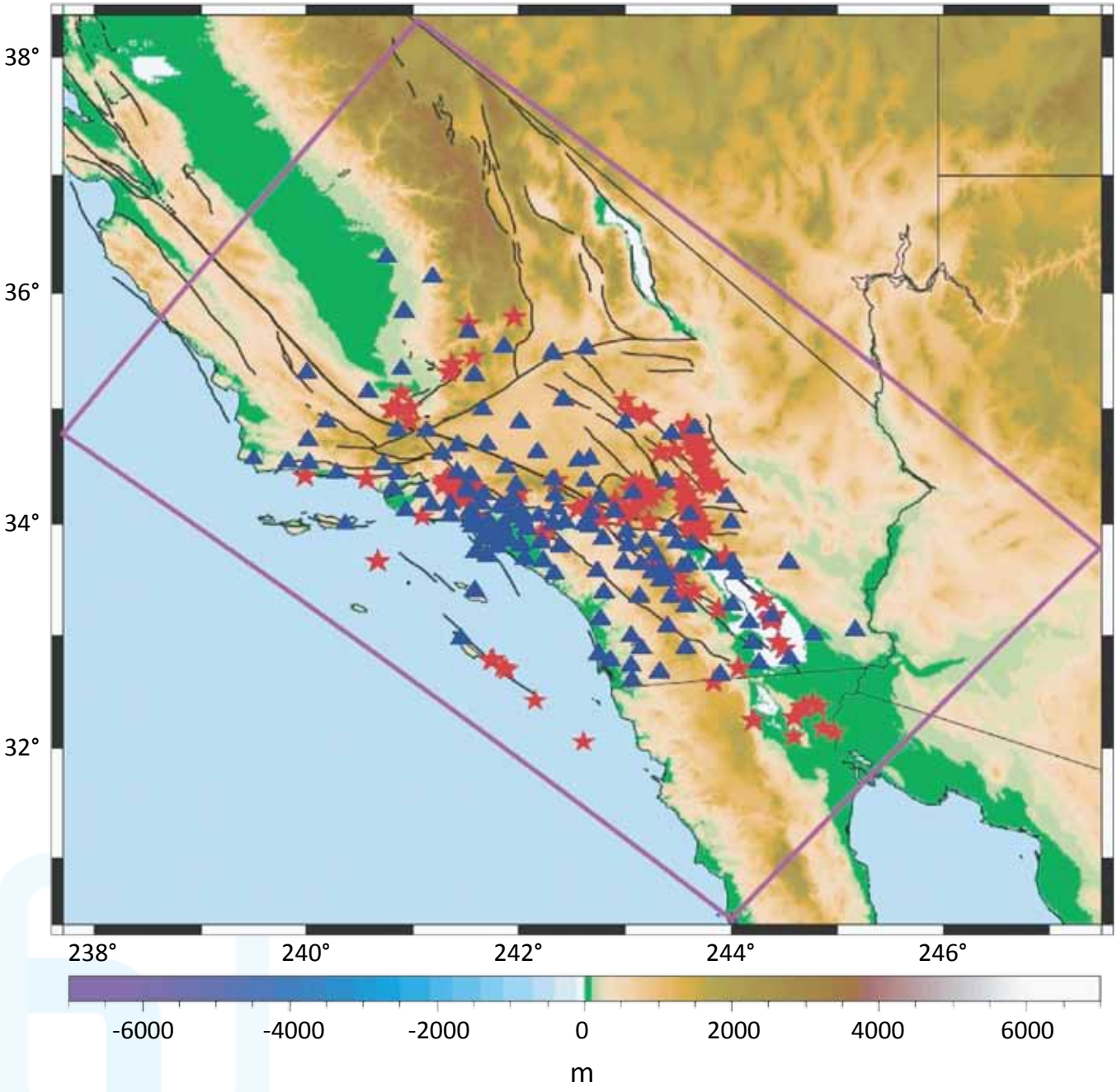
INCITE Hours Allocated on the ALCF's Blue Gene/P: 5 Million

Deterministic Simulations of Large Regional Earthquakes at Frequencies up to 2Hz

Earthquake simulations help scientists understand the hazards posed by large future earthquakes. Before predictive simulation results for future earthquakes are scientifically acceptable, the earthquake computational models must be validated by simulating well-recorded historical earthquakes and comparing simulation results to observational data.



The purple border shows the extent of the 3-D structural model used in the 3-D inversion. Events in red, with stations in blue. (Image Credit: En-Jui Lee, University of Wyoming)

Scientific Approach

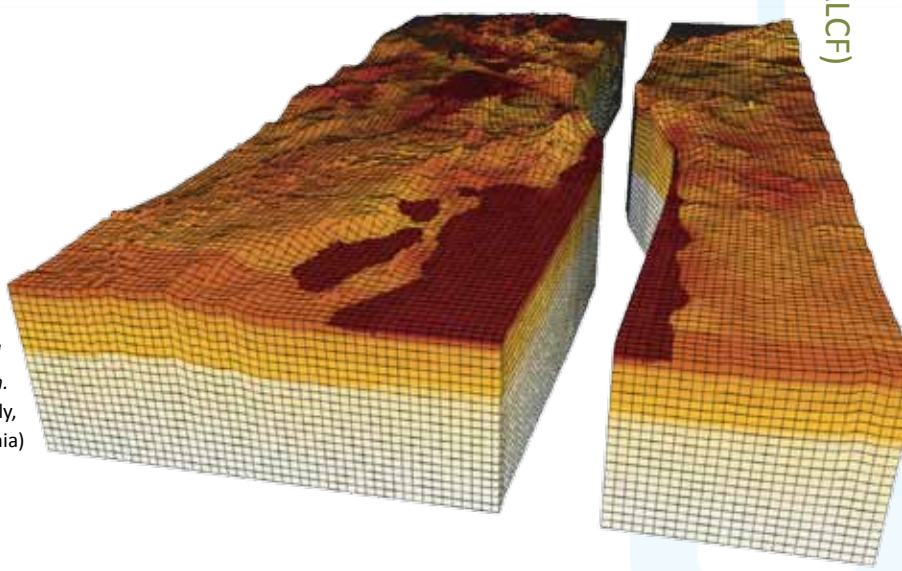
SCEC researchers used the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF) to simulate nearly 150 historical Southern California earthquakes. Simulation results were compared against observational seismograms to confirm that the SCEC simulation codes and 3D structural model for California accurately reproduced the observed ground motions.

Results

This large-scale validation work was performed as part of a scattering integral (SI) 3-D-inversion that validated the SCEC simulation code and the 3-D structural model of California and produced an updated and improved 3-D structural model. The improved 3-D model will be used in future high-resolution earthquake simulations because it produces a better fit between simulation and observation.

Future Efforts

The computational requirements for SCEC earthquake simulations increase each year as scientists simulate earthquake processes at higher frequencies. They utilize an iterative process of improvement as they scale up the computational model that includes simulation of historical earthquakes, validation against observation, 3-D structural model optimization, and then simulation of large future earthquakes.



This shows the 3-D structural model for Southern California and how the model is discretized for use in a simulation.
(Image Credit: Geoffrey Ely, University of Southern California)

INCITE Contribution

"The INCITE program immediately understood the importance of this validation work and supported our efforts in numerous ways. We would not have completed our 3-D-inversion this year without the INCITE award."

ALCF Contribution

"The outstanding resources at the Argonne Leadership Computing Facility enabled us to perform a regional-scale 3-D inversion of southern California two or three times faster than our earlier efforts on other open-science HPC systems. The high productivity we experienced using ALCF has raised the ambitions of the SCEC simulation group and has enabled us to increase the computational scales at which we are running."

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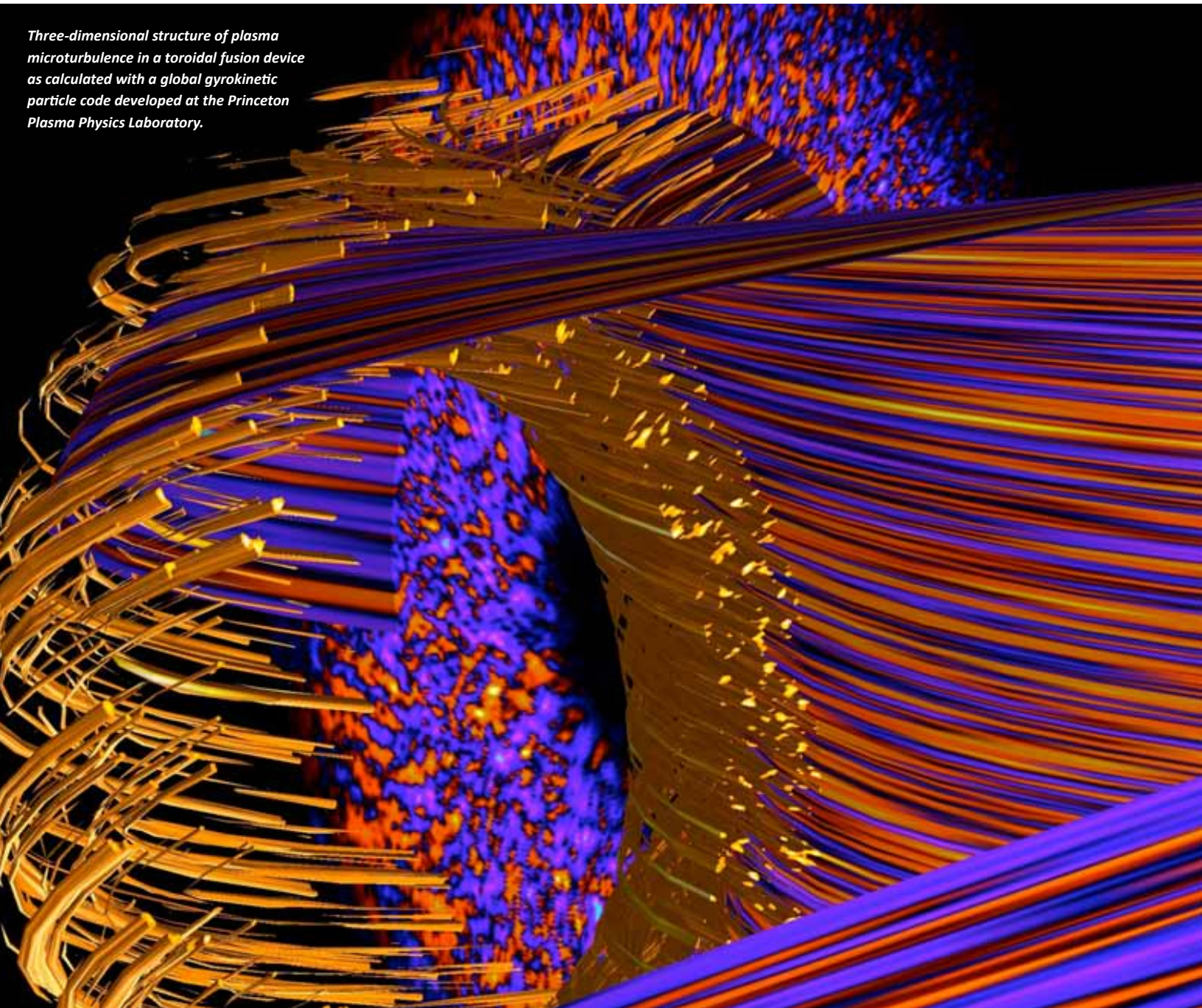
INCITE Hours Allocated on the ALCF's Blue Gene/P: 6 Million

How Can Scientists Control Microturbulence to Make Nuclear Fusion More Efficient?

As the global energy economy shifts its focus from fossil fuels toward cleaner alternatives, nuclear fusion is an increasingly attractive possibility for meeting our growing energy needs. Fusion, the power source of the sun and other stars, has been the focus of researchers since the early 1950s. While progress has been impressive, scientists have yet to solve the problem of microturbulence—the key means by which heat leaks out of the magnetic trap designed to confine the hot plasma gas. Understanding and controlling such losses is key to achieving the efficiency needed to help ensure the practicality of fusion power plants.



Three-dimensional structure of plasma microturbulence in a toroidal fusion device as calculated with a global gyrokinetic particle code developed at the Princeton Plasma Physics Laboratory.

Scientific Approach

Use of predictive computational models derived from first-principles physics equations has allowed for unparalleled gains in our knowledge of microturbulence. Scientists from the Princeton Plasma Physics Laboratory have developed the advanced 3-D global, particle-in-cell code GTC and optimized it using the IBM Blue Gene/P quad-core LCF to conduct a realistic examination of the effect of collisions on the plasma confinement properties. The multi-core processors of the Blue Gene/P allow for higher-resolution simulations in a multi-dimensional phase-space. With this unprecedented capability, advanced kinetic simulations with higher physics fidelity can be directly applied for the interpretation of experimental results. This, in turn, will pave the way for future scientific discoveries needed for accelerating progress toward the goal of peaceful, benign, and essentially inexhaustible fusion power.

Results

The science results achieved to date in this INCITE project have demonstrated that high-resolution global simulations of plasma microturbulence, which take into account the presence of previously neglected collisional dynamics, can be successfully carried out on the IBM Blue Gene/P architecture. These long-time simulations not only provide evidence that collisional dynamics cannot be ignored but that a larger number of particles per cell is necessary to achieve the phase-space resolution needed. In addition, preliminary diagnosis of the turbulent energy spectra produced in these simulations provides evidence that there exists a nonlinear inverse cascade into the longer wavelength regime. Such insights enhance the knowledge base needed for understanding and then mitigating the influence of microturbulence on efficient magnetic confinement of fusion-grade plasmas.

Future Efforts

Researchers will examine the key question of how the trends observed in the current simulations might be affected as plasma size increases from that of existing experiments to the future very large plasmas characteristic of ITER. They will have the ability to systematically address this challenging issue with a new radial domain decomposition capability that has recently been successfully implemented into their code.

INCITE Contribution

"The INCITE award enabled systematic runs demonstrating the improved efficiency of the new hybrid (OpenMP/MPI) approach implemented into GTC over that of the code run with MPI alone on BG/P. It has also supported valuable developmental activities, which have positioned the project very well to move forward with production runs. We have captured important information on ITER-scale plasmas with unprecedented resolution in a multi-dimensional phase-space to deliver scientific results appropriate for 'path to petascale' grand challenges."

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING

ALCF Contribution

"The ALCF staff has been very helpful in the implementation of our code on the quad-core BG/P. We are grateful for the support provided to set up process mapping for the GTC simulations. This has resulted recently in a 14% improvement in performance by simply using a mapping file that best matches our communication patterns to the physical configuration of the BG/P interconnect."

Contacts

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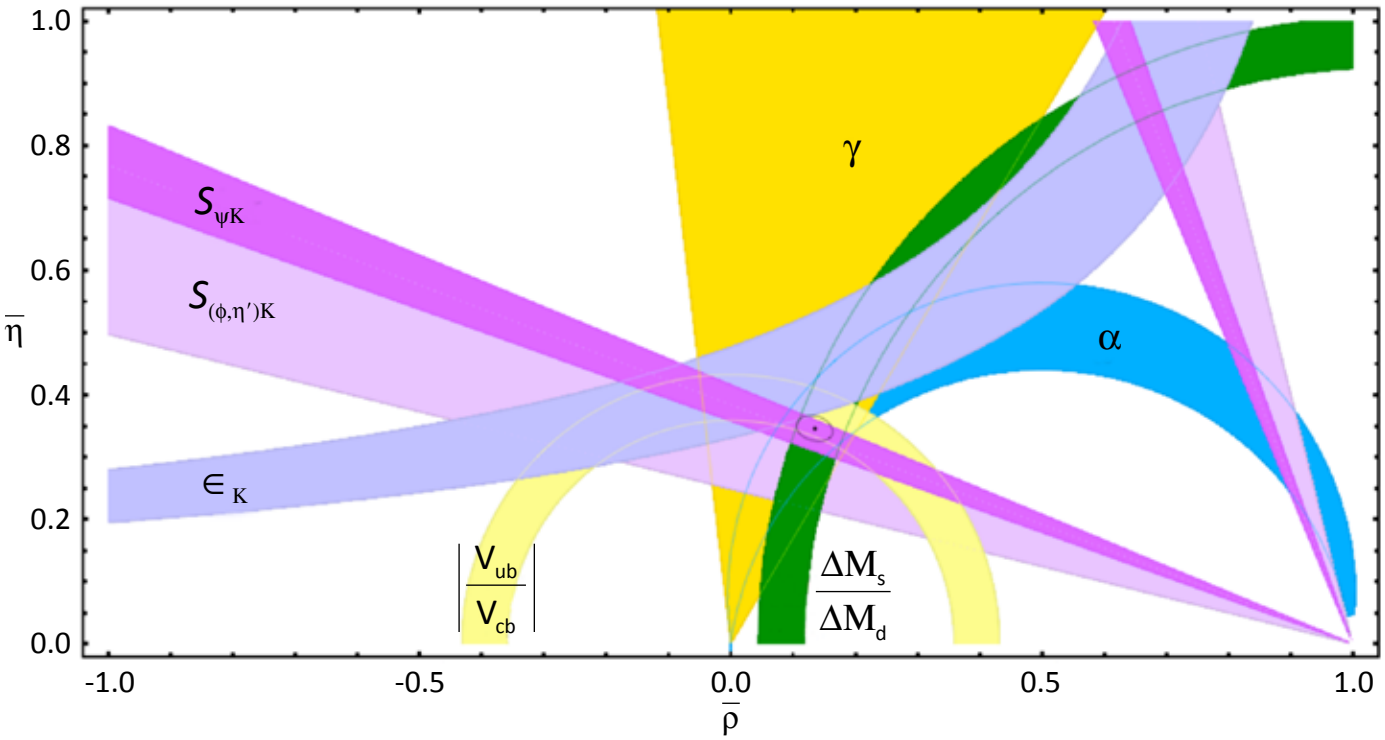
INCITE Hours Allocated on the ALCF's Blue Gene/P: 67 Million

How Can We Better Understand the Basic Building Blocks of Nature?

Scientists have long sought to understand the basic building blocks of nature. While the behavior of particles such as protons and neutrons is well understood, less is known about the behavior of quarks and gluons, the even-smaller particles that make up protons and neutrons. Because they interact very differently than larger particles, the study of interactions between quarks and gluons, Quantum Chromodynamics (QCD), requires different methodology. With the help of supercomputers, scientists use a four-dimensional lattice representation of space-time to analyze QCD.

This research aims to deepen the understanding of the interactions of quarks and gluons, the basic constituents of 99 percent of the visible matter in the universe. It will play a key role in ongoing efforts to develop a unified theory of the four fundamental forces of nature.



The lattice QCD calculations performed of the decays and mixings of strongly interacting particles enable increasingly precise determinations of the parameters of the Standard Model of particle physics. This figure shows the bounds on the CP violating parameters rho *and* eta *obtained from the mixings of K and B mesons with their antiparticles and from the decay of a B meson into a pion plus leptons.*

INCITE Contribution

"The INCITE award at the ALCF made possible the creation of ensembles of improved-staggered and domain-wall gauge configurations with the smallest lattice spacings and the lightest quark masses that had ever been made. These ensembles are playing an important role in the accurate determination of a wide variety of physical quantities."

Scientific Approach

Scientists conducting QCD research have logged over 300 million core hours on the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF). The scientists have generated gauge configurations with up, down, and strange quarks on lattices that are sufficiently fine-grained and have sufficiently small up and down quark masses to enable the extrapolation of key quantities to their physical values found in nature. The gauge configurations are being used to determine a wide range of important physical quantities in high energy and nuclear physics.

Results

With the use of the Blue Gene/P, the generation of gauge configurations has been accelerated in many cases by a factor of 5 to 10 over what has been possible with other machines.

Domain-wall configuration ensembles of lattice spacings 0.114 femtometers (fm) and 0.086 fm have been completed on lattices of sizes 24^3x64 and 32 x64, respectively. These are the largest domain-wall lattices ever attempted. For the staggered quarks, a set of runs with a lattice spacing of 0.06 and 0.045 fm have been completed. These are the most challenging staggered ensembles generated to date.

These ensembles are currently being analyzed at the ALCF and elsewhere in studies of the decays and mixings of particles containing heavy quarks to enable major improvements in determining a number of elements of the CKM matrix. These calculations are enabling precise tests of the Standard Model, aiding in a deeper understanding of fundamental physics.

Future Efforts

Improved versions of both methods for lattice fermions are currently being completed. For domain-wall fermions, a new method has been developed (the "AuxDet" method) that will permit a closer approach to the physical, light quark limit. For staggered fermions, an improved discretization method has been developed ("hisq" fermions) that substantially reduces discretization errors. New ensembles with the improved methods are expected in the coming year.

USQCD Collaboration.

ALCF Contribution

"Our ALCF liaison, James Osborne, has provided extraordinary assistance. He has played an important role in the success of our work on the Blue Gene/P."

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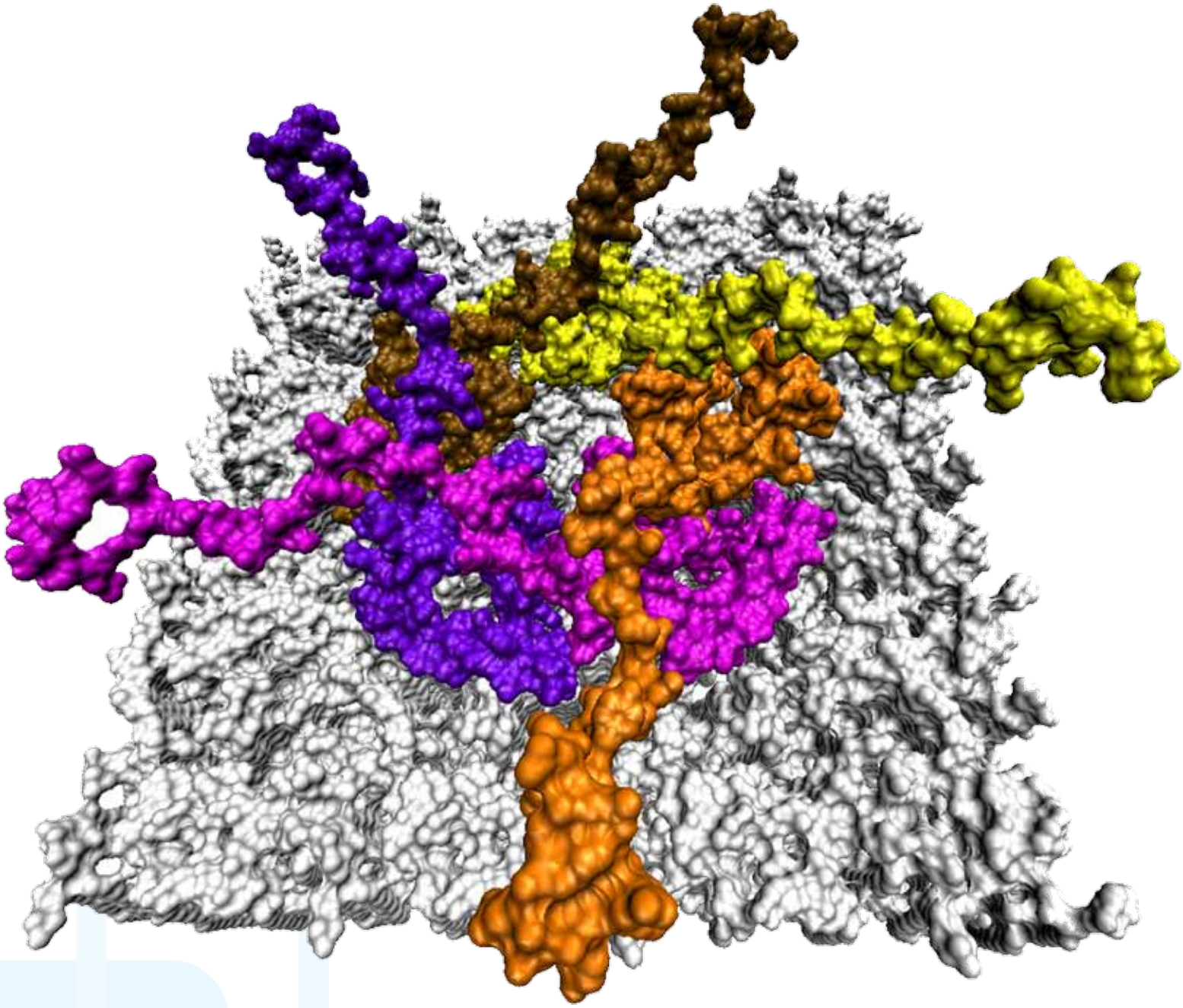
INCITE Hours Allocated on the ALCF's Blue Gene/P: 3 Million

Modeling the Molecular Basis of Parkinson's Disease

As the second most common neurological disorder in adults, the personal and economic impacts of Parkinson's disease are enormous. Currently, there are more than 2 million cases in the United States. In economic terms, the disease exacts an annual cost of $25 billion on the U.S. economy alone.



Alpha-synuclein pentamer on the membrane. The pentamer is constructed with theoretical docking of Asyn conformers that occur at 4 ns of MD simulation. These conformers have the best membrane contacting properties (calculated by the program MAPAS). The geometrical dimensions of this pentamer correspond to the experimentally elucidated by electron microscopy.

Scientific Approach

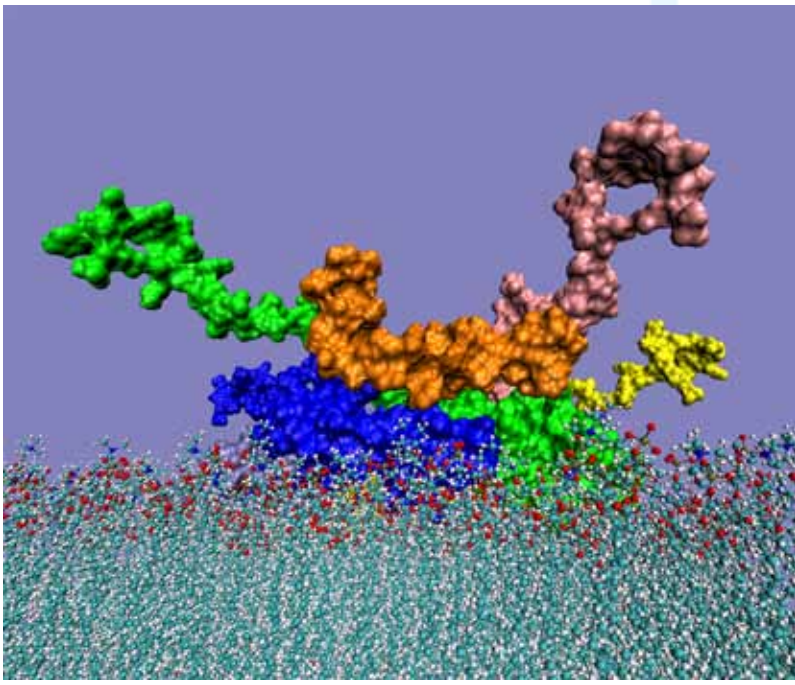
University of California—San Diego scientists have shown that the clumping of a protein known as alpha-synuclein (aS) in the brain can lead to harmful, pore-like structures in human membranes. In contrast, another protein, beta-synuclein (bS), appears to block the clumping action. Researchers are leveraging the high-end computation power of the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF) to learn more about the molecular basis of the disease and to explore ways to treat it.

Results

Research is providing insights into the molecular mechanism for Parkinson's disease progression and will have broad applicability to other diseases. The findings also provide a test bed for identifying possible therapeutic interventions through computational modeling. Given the encouraging correlation between the molecular dynamics modeling predictions and laboratory experimental results, the team expects to make steady progress both with the computational model itself and with the design of effective drugs based on the computational modeling and simulations.

Future Efforts

The research team will focus on a more comprehensive investigation of alpha-synuclein penetration into the membrane, including a thorough study of pore creation. The scope of the team's work has increased in both the number of simulations being conducted and the scale of the simulations.



Alpha-synuclein (Asyn) pentamer (various colors for each participating Asyn molecule) on the cell membrane interacting with beta-amyloid 1-42 (Abeta) [orange]. This interaction can contribute to neurodegeneration during the combination of Parkinson's and Alzheimer's diseases.

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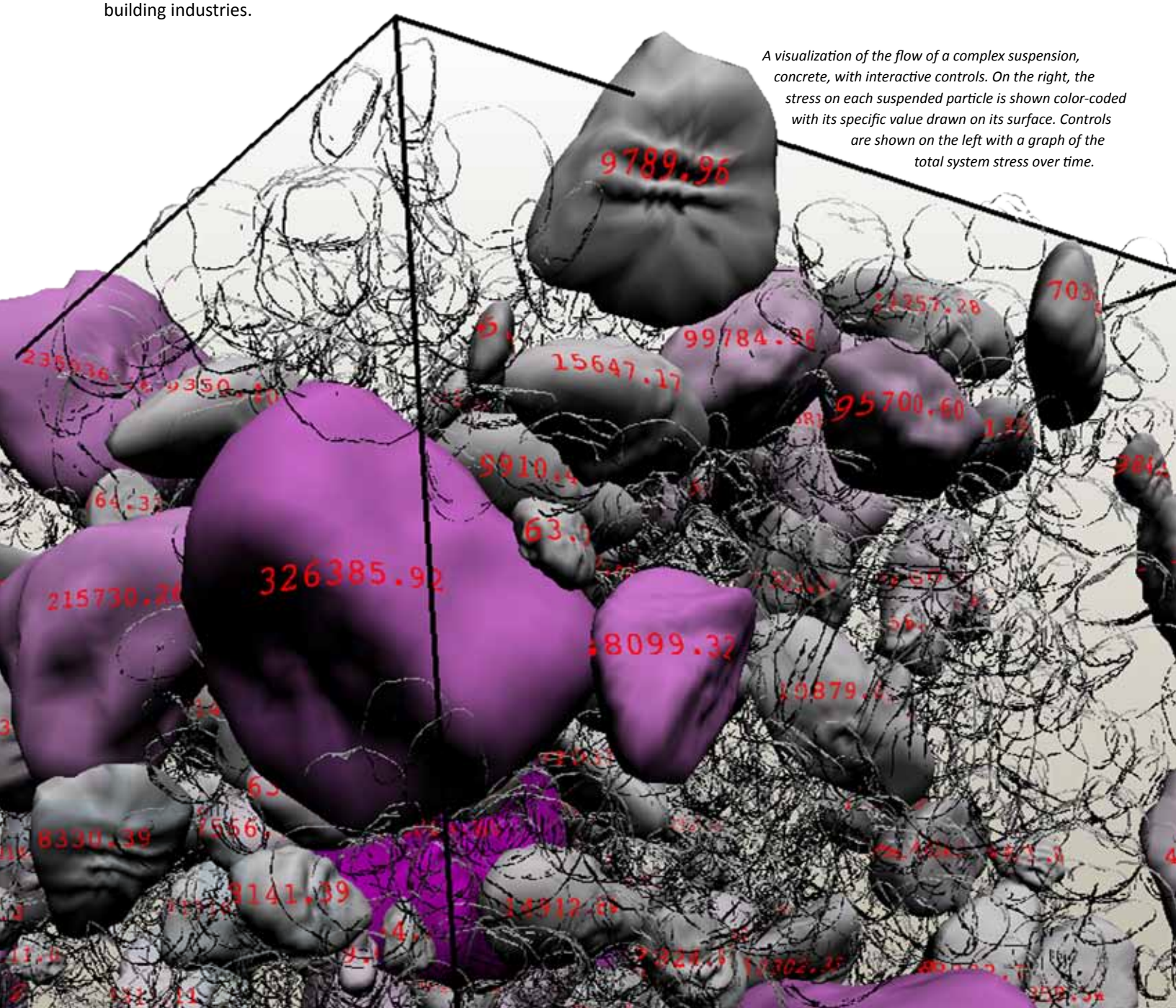
INCITE Hours Allocated on the ALCF's Blue Gene/P: 750,000

What Insights Are Revealed When Modeling Concrete's Rheological Properties?

Study of the flow behavior of dense suspensions remains an outstanding research problem because of the immense complexity of these systems that are not tractable by simple analytic theories. Computational models are needed that account for dense packing of particles with a broad shape and size variation along with interparticle interactions. Researchers from the National Institute of Standards and Technology are leveraging the computational resources of the Blue Gene/P at the Argonne Leadership Computing Facility to shed light on the mechanisms for the dispersion or agglomeration of suspensions. Insight from these studies has technological application in a wide variety of areas, including pharmaceuticals, foods, coatings, and building industries.



A visualization of the flow of a complex suspension, concrete, with interactive controls. On the right, the stress on each suspended particle is shown color-coded with its specific value drawn on its surface. Controls are shown on the left with a graph of the total system stress over time.

Scientific Approach

This project focuses on the flow of dense suspensions and related colloidal systems composed of rigid bodies, with and without interparticle interaction, having a wide range of size and shape, and under a variety of flow conditions such as shear and around obstacles. The computational approach is based on a modified Dissipative Particle Dynamics (DPD) model, which includes lubrication and Van der Waals forces for different shape particles near contact. The DPD model has been extended to model suspensions with a non-Newtonian fluid matrix—allowing researchers to scale up suspension simulations with particles ranging from m sized (cement) to cm sized (aggregate).

Results

Preliminary studies by the group indicate that particle contacts are an important factor in controlling the onset of flow in dense suspensions. Also, for the case of suspensions with a non-Newtonian fluid matrix, the local shear rates between aggregates strongly determine their rheological properties. These results have been validated against physical experiments with excellent agreement.

Future Efforts

Research plans include studying the effect of varying particle shape, by mixing different classes of particles that are representative of realist materials, and comparing the effect of Newtonian vs. non-Newtonian fluid matrices on the rheological behavior of suspensions.

INCITE Contribution

"Our simulations on Intrepid have helped shed light on physical mechanisms that control the onset of flow in dense colloidal suspensions."

ALCF Contribution

"Access to the compute power in the ALCF, specifically the IBM Blue Gene/P, has allowed us to systematically probe regimes that are more representative of real physical systems than is possible on other compute resources available to us."

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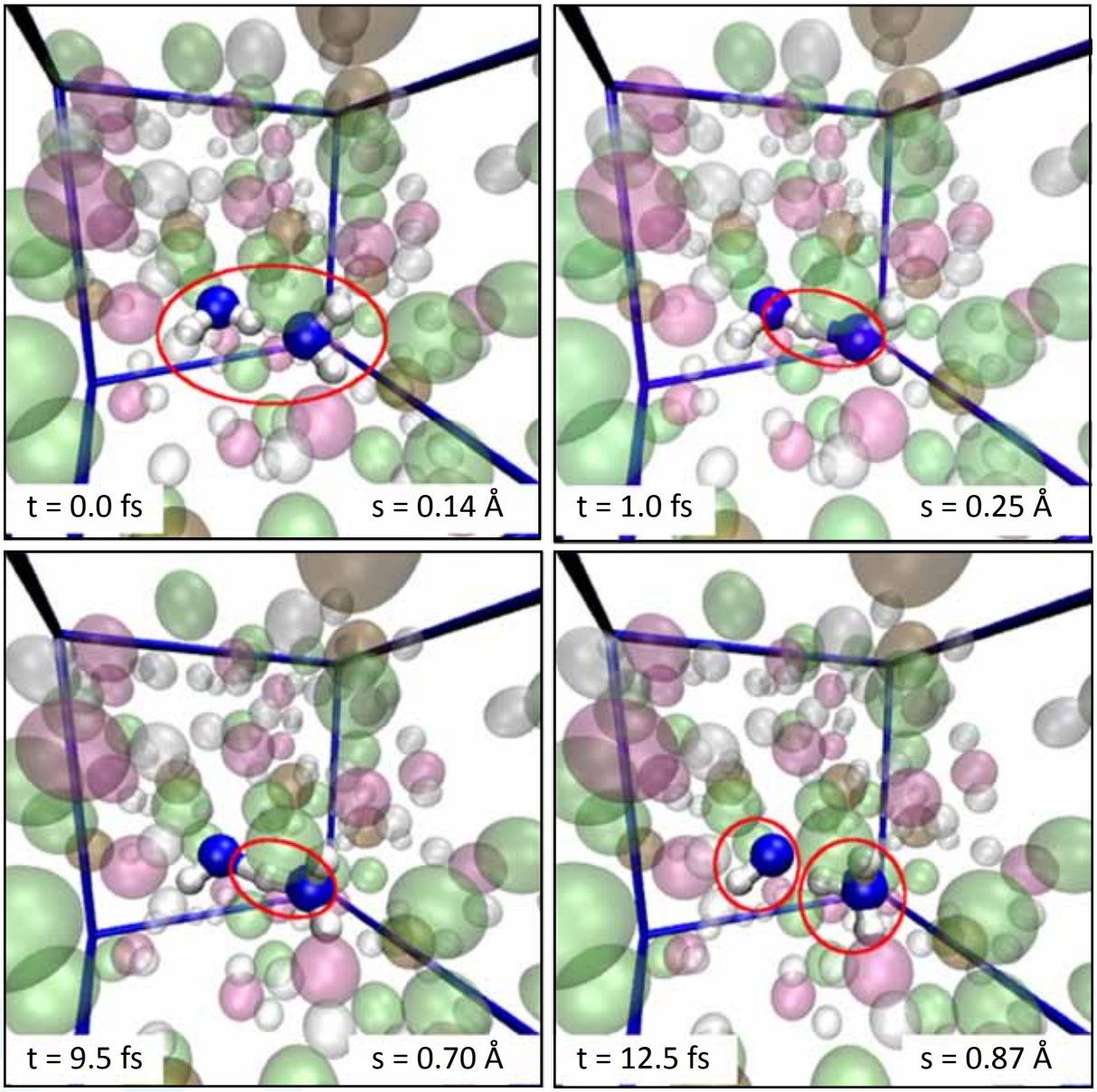
INCITE Hours Allocated on the ALCF's Blue Gene/P: 1 Million

Accelerating the Pace of Discovery in Alternative Fuels Research

Scientists continue to seek clean, renewable energy sources that will reduce the nation's dependence on foreign oil. One promising, possible energy source for cars is hydrogen. However, to make hydrogen a viable power solution, scientists must find a two-pronged solution: They must find practical ways to first store the hydrogen onboard the vehicle and to then extract the energy back out of its stored state for use. Though researchers have identified ways to safely store hydrogen within other materials, currently available materials are typically either much too heavy or else bind the hydrogen within the material much too strongly. Quickly extracting energy back out of those materials requires extremely high levels of heat—impractical for actual use in vehicles on the open road.



Snapshots of configurations during NH3 formation reaction in $Li_4BN_3H_{10}$ at 1000K from Ab-Initio *Molecular Dynamics. The reaction coordinate, s, was defined as the distance between the "hopping" hydrogen traveled. INCITE resources allow researchers to simulate ensembles, including hundreds of members to obtain statistics on chemical reactions, structure, and energetics that will guide hydrogen storage decisions.*

Scientific Approach

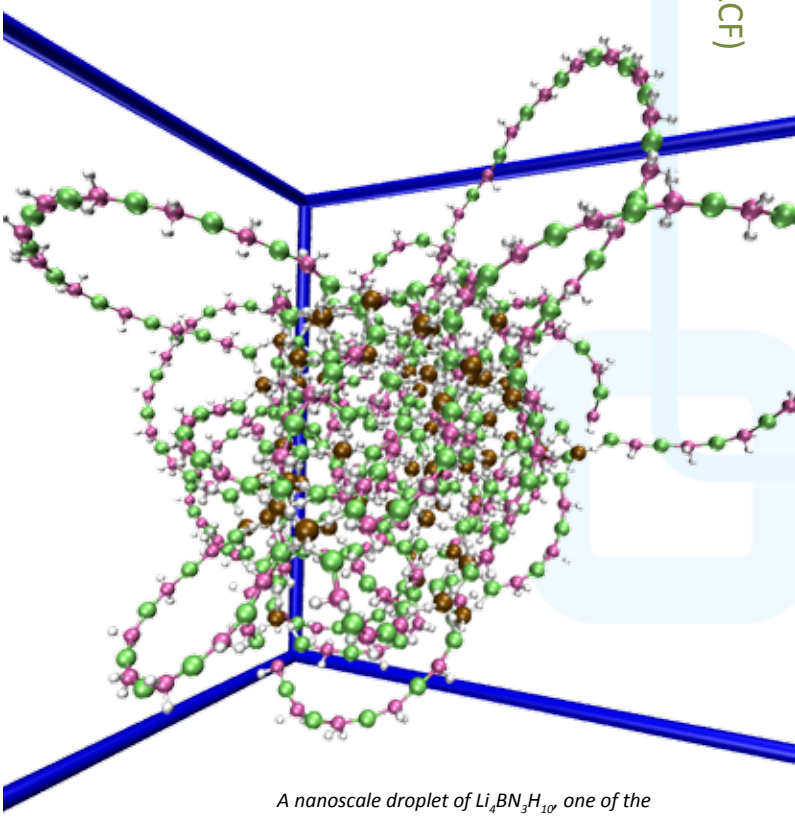
By creating a suite of computational tools for use on the massive compute power of the Argonne Leadership Computing Facility (ALCF), a research team from Northwestern University and UCLA will create a "virtual laboratory." Here, a predictive, physics-based modeling approach will allow possible storage materials to be constructed and tested, all on computers, before they are ever synthesized in a laboratory, thus rapidly accelerating the pace of discovery.

Results

This research has broad implications for a wide variety of alternative energy technologies, including battery electrodes, solar electricity cells, thermoelectrics, and fuel cells. For each, computation will play a key role in facilitating new discoveries.

Future Efforts

Researchers now turn their attention to the realm of kinetics, which dictate the rates of hydrogen release (and reinsertion) from materials. Scientists will use the accurate predictive power of first-principles modeling to understand the microscopic kinetic processes involved in the hydrogen release and uptake. That information will aid in the design of new systems with improved properties. Specific areas of study will include the fundamental factors that control hydrogen-metal bond strength, the role of surface structure and finite size on the thermodynamics and kinetics of hydride nanoparticles, and the effect of dopants and nanoscale catalysts in achieving fast kinetics and reversibility at the atomic level.



A nanoscale droplet of $Li_4BN_3H_{10}$, one of the configurations researchers are studying via Ab-Initio *Molecular Dynamics to better understand the kinetics of hydrogen release in complex hydrides.*

INCITE Contribution

"Our calculations require state-of-the-art first-principles molecular dynamics simulations, using a very large system size (i.e., thousands of atoms) and a very long simulation time. The types of atomic-scale kinetic calculations we are undertaking are simply impossible without the large-scale computing resources generously made available through the Department of Energy's INCITE program."

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

ALCF Contribution

"The ALCF has been extremely helpful in guiding this work towards a more efficient use of their Blue Gene machine and providing important information about new codes with better scaling behavior over large numbers of processors than some of the standard computational tools we would have used. Their continued assistance will be critical in moving this project forward."

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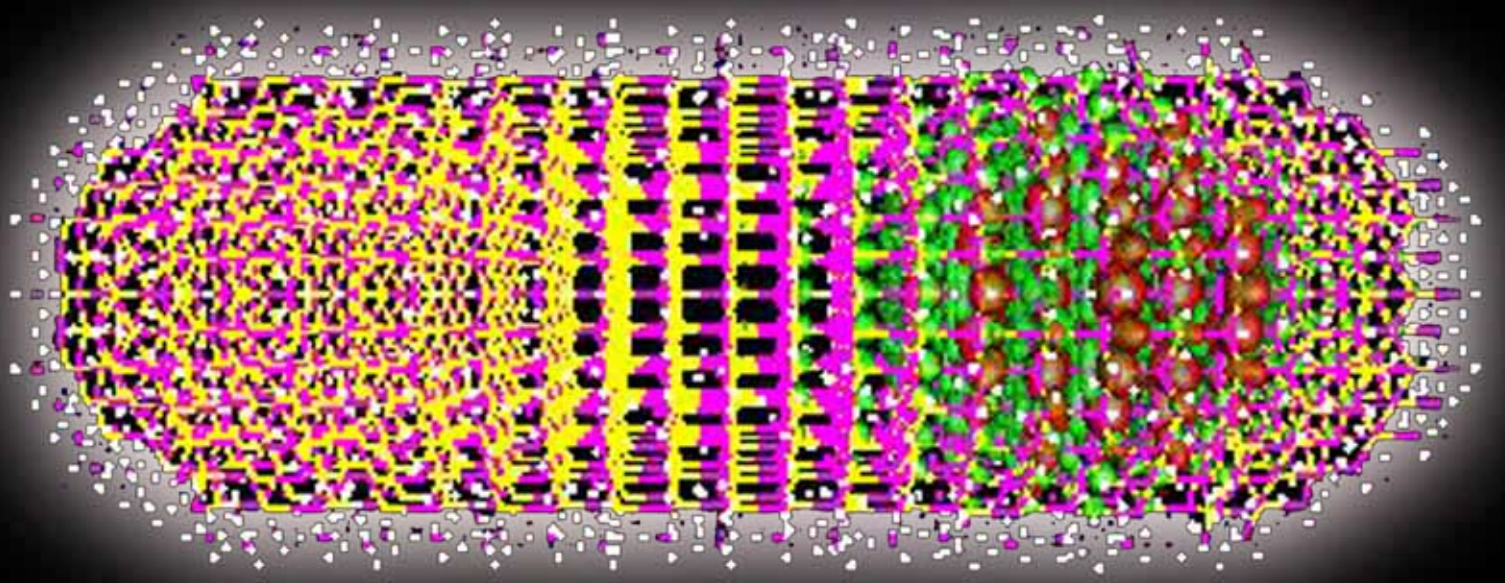
INCITE Hours Allocated on the ALCF's Blue Gene/P: 1 Millioin

Why Are Nanomaterials Promising for Solar Cells?

Widespread use of solar cells is precluded by the high cost and poor efficiency of conventional solar cell technology. Scientists believe that nanomaterials are a promising candidate for achieving greater solar energy deployment. However, it is first necessary to understand the internal electric field in these nanostructures, caused either by bulk and surface dipole moments, or piezoelectric effects.

A CdSe/CdS core/shell nanorod calculated by the LS3DF code. Such nanorods have the potential to be used in solar cell applications. The green isosurface is the electron state, while the dark red isosurface is the hole. The CdSe core is located at the right-hand side, near the hole.



Scientific Approach

A "divide-and-conquer" *ab initio* method implemented in the LS3DF (Linear Scaling Three-Dimensional Fragment) code is used to calculate the charge density and electric field inside a 5,000-atom nanostructure. Researchers are able to run the LS3DF code using tens of thousands of processors on the Blue Gene/P at the Argonne Leadership Computing Facility (ALCF).

Results

As a result of their work, surprisingly large electric fields have been discovered in nanorods, often caused by dipole moments from the side surfaces. Such electric fields will completely separate the electron and hole to opposing sides of the nanorod. Scientists also have determined that the piezoelectric effect is relatively small.

Future Efforts

In the next phase of this project, researchers will relax the atoms using LS3DF to search for charge compensation mechanisms that would counterbalance the internal electric fields in these nanorods.

INCITE Contribution

"Without the INCITE award, we would never be able to carry out such large-scale computation. It has enabled us to understand better the electric field in a nanostructure and has revealed to us the surprises in the nano-world."

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ALCF Contribution

"The ALCF staff has helped us to analyze the code and to overcome bottlenecks for improved performance. Access to machines like Intrepid enables us to calculate large systems that could not be studied before."

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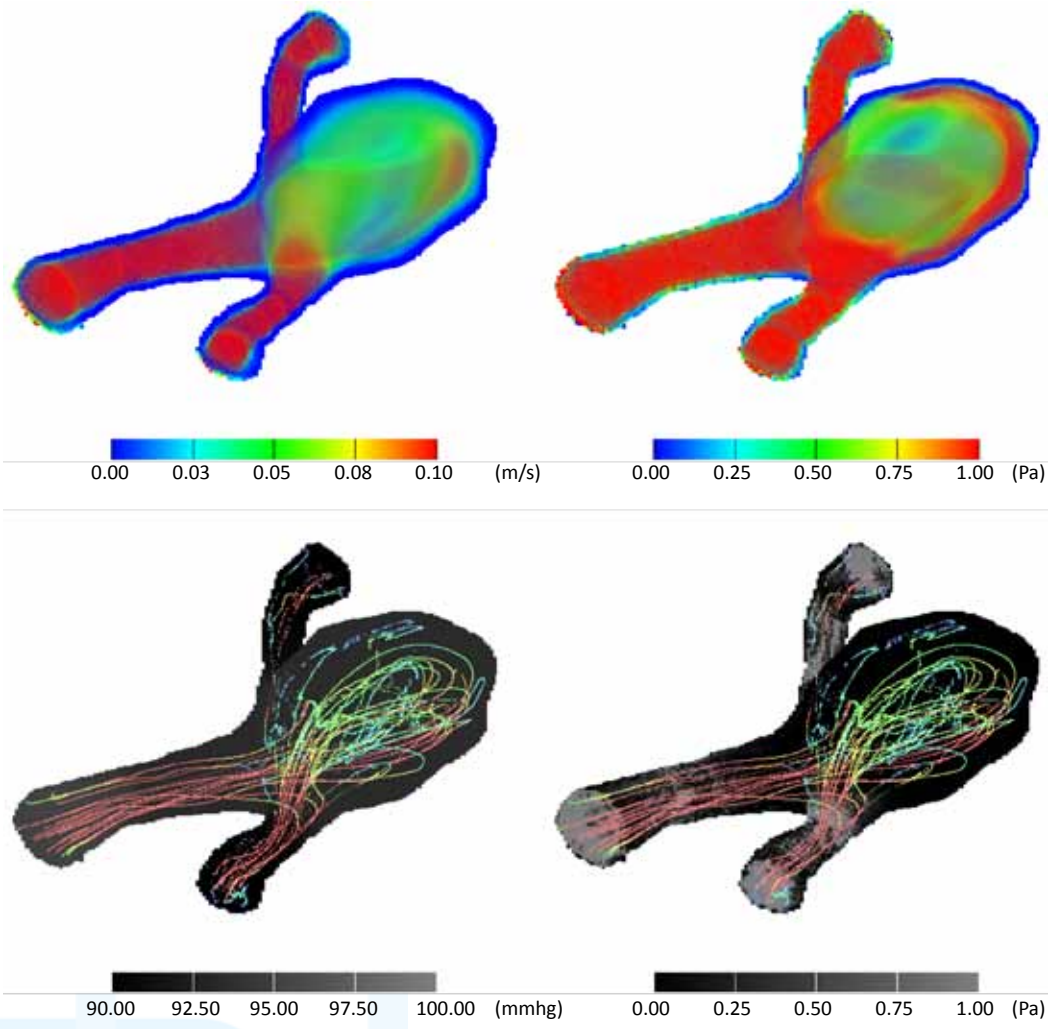
INCITE Hours Allocated on the ALCF's Blue Gene/P: 40 Million

Cerebral Blood Flow Behavior Helps Scientists Understand Cardiovascular Disease (Part I)

Large-Scale Condensed Matter and Fluid Dynamics Simulations in Three Diverse Areas

Part I: Whole Brain Blood Flow Simulations

Cardiovascular disease is the third largest cause of death in the developed world. Cerebral blood flow behavior plays a crucial role in understanding, diagnosing, and treating the disease, where problems are often due to anomalous blood flow behavior in the neighborhood of bifurcations and aneurysms within the brain.



The figure depicts a snapshot of blood flow simulated and visualised using the parallel LB code HemeLB within a digitally reconstructed patient-specific middle cerebral artery aneurysm. The top-left and top-right images show the volume rendering of the velocity field and of the stress respectively. The greyscale distribution shows blood pressure (bottom-left image) and stress (bottom-right image) at the inner surface of the aneurysm and surrounding blood vessels. The particle traces within the vasculature are colored according to the local velocity, effectively illustrating blood flow motion and portraying vortex fluid flow features.

Scientific Approach

Using computer simulations, scientists and clinicians will conduct virtual experiments to study cerebral blood flow at the individual patient level, resulting in customized patient blood-flow simulations.

Having a computational tool surgeons can use, not only to examine the pressure and velocity variations through an individual's vasculature, but also to predict what changes might occur as a result of interventional surgery, will be an invaluable addition to the surgical tool kit. Because patient-specific data is used as the basis of the simulation, treatments can be assessed for their effectiveness with respect to the individual before being administered, thus reducing risk and expense.

Results

Researchers are focusing on two types of aneurysms which occur in different vessels in the brain—internal carotid artery aneurysms and pericallosal artery aneurysms. Investigations are looking at patients to find relationships between the formation of these aneurysms and their overall brain artery structure.

Future Efforts

Improvements to the computational model will make vessel walls elastic. The result is a far more realistic model of how blood flows through the brain.

INCITE Contribution

"As displayed by each of the three main projects' synopses, the results obtained so far would not have been possible without the INCITE award that was generously awarded to our group. We aim to pursue the paths outlined here and to continue pushing the envelope in terms of scientific, large-scale computing and visualization."

ALCF Contribution

"We are very grateful for the contribution of the whole ALCF team, in all stages of this work. This includes the porting, benchmarking, and optimization of our large-scale parallel codes on the IBM Blue Gene/P machine, as well as use of the team's liaison and outreach facilities. In all these aspects, the support of ALCF has been invaluable!"

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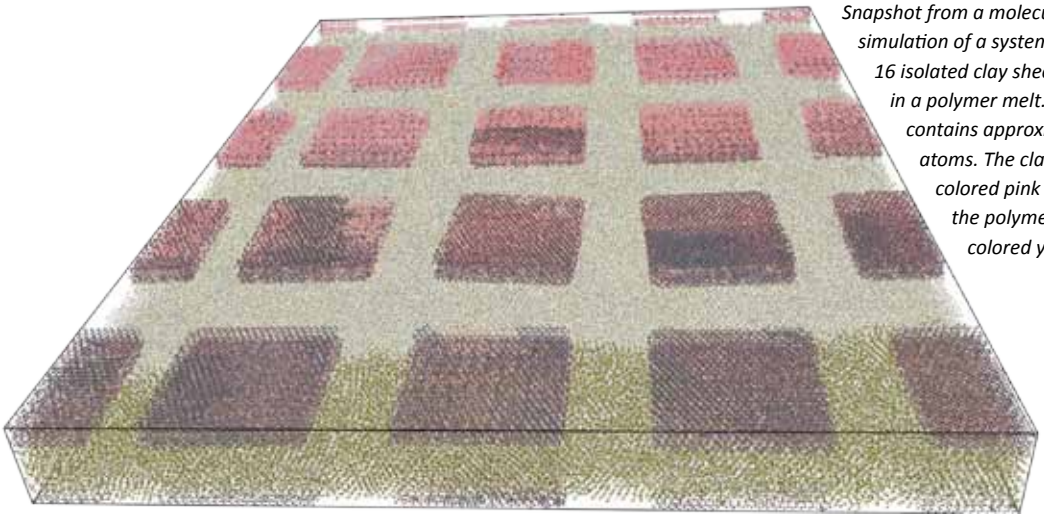
INCITE Hours Allocated on the ALCF's Blue Gene/P: 40 Million

Cerebral Blood Flow Behavior Helps Scientists Understand Cardiovascular Disease (Part II)

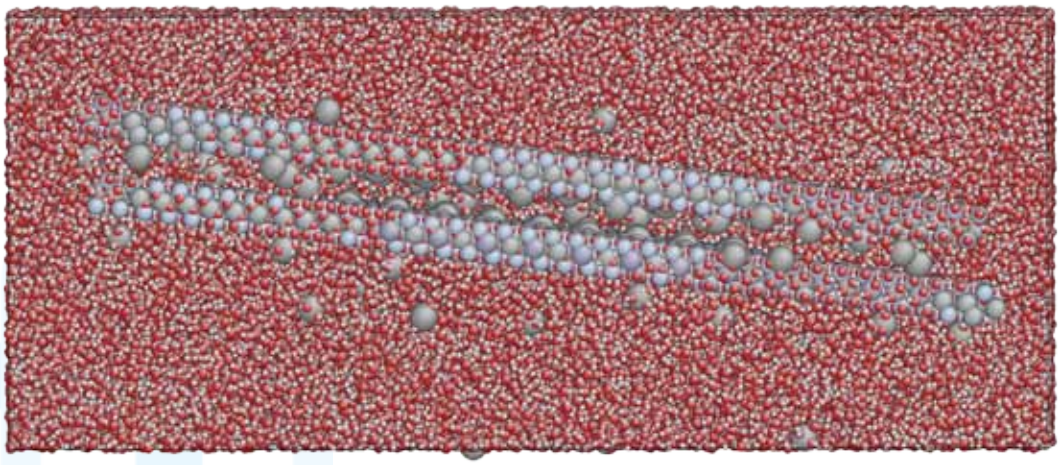
Large-Scale Condensed Matter and Fluid Dynamics Simulations in Three Diverse Areas

Part II: Molecular Dynamics Study of Clay-Polymer Nanocomposites

We use large-scale molecular dynamics simulations combined with rare event sampling techniques to understand the unique chemical and physical aspects associated with clay-polymer-based nanocomposite materials. Tailoring the clay structure in polymers on the nanometer scale produces composites with novel material properties that have already been applied in numerous commercial applications. Once fundamentally understood, clay-polymer nanocomposites have the potential to become as widespread as traditional, conventional composite materials.



Snapshot from a molecular dynamics simulation of a system containing 16 isolated clay sheets immersed in a polymer melt. This system contains approximately 3 million atoms. The clay atoms are colored pink and brown; the polymer atoms are colored yellow.



Snapshot from a molecular dynamics simulation of an isolated clay platelet (consisting of two sheets) immersed in water. Note the water diffusing through the interlayer spacing. The oxygen atoms are colored red, hydrogen atoms are white, sodium atoms are dark grey, clay atoms are light blue and light grey.

Scientific Approach

Researchers will perform non-equilibrium molecular dynamics (NEMD) simulations of clay-polymer nanocomposites, from which they will calculate material properties. The scale of the systems involved allows, for the first time, study of the arrangement of discrete platelets in atomistic detail.

Using a parallel tempering technique (replica exchange), scientists will simulate polymer penetration into the clay platelet, a process that occurs on a time scale outside that possible with a single molecular dynamics simulation. A greater understanding of the mechanism of intercalation in these materials will lead to improved techniques for nanocomposite formation.

Thirdly, researchers will generate coarse-grained representations of the clay platelets using the atomistic simulations of interaction parameters between the coarse-grained superatoms. Coarse-grained simulations are expected to be achieved in micro- to milliseconds.

Results

To date, scientists have created clay-polymer nanocomposite systems consisting of approximately 10 million, containing 16 isolated clay platelets–the first time such simulations of isolated platelets have been run. They have performed molecular dynamics simulations using the LAMMPS code up to a simulation time of 1ns, which is currently being extended, and will form the basis of elastic calculations to further understand the properties of clay-polymer nanocomposites. A smaller system consisting of a single platelet immersed in water allows researchers to understand the process of intercalation of small molecules into the interlayer spacing between clay sheets. It will be the basis for the parallel tempering technique, which will be used to study similar, but much rarer, intercalation of large polymer molecules.

Scientists have also developed a protocol for building coarse-grained simulation from all-atom simulations, from which we have built a test system of 500,000 coarse-grained particles, which corresponds to a 4 million atom system.

Future Efforts

Moving forward, researchers will perform NEMD simulations of the clay-polymer nanocomposites, from which they will calculate material properties, including the bending modulus, Young's modulus, and Poisson's ratio. The objective is a greater understanding of the enhancement mechanism, which may be a cooperative effect over the many disparate length scales. They will also be able to study the interactions between separate platelets, which may determine the rheology of clay nanocomposites. In addition, scientists will ascertain how the long-range order and arrangement of the platelets affect the material properties of the nanocomposites. Because of the sheer scale involved, no previous study has ever considered the arrangement of discrete platelets in atomistic detail.

Their coarse-grained simulations will allow exploration of greater time-scales than possible with atomistic molecular dynamics, providing another avenue to explore the intercalation mechanism and long-range order. From the biological domain, researchers expect their coarse-grained simulations to allow speed-ups of many orders of magnitude. Further, they expect their coarse-grained simulations to be achieved in micro- to milliseconds, approaching realistic synthesis time scales.

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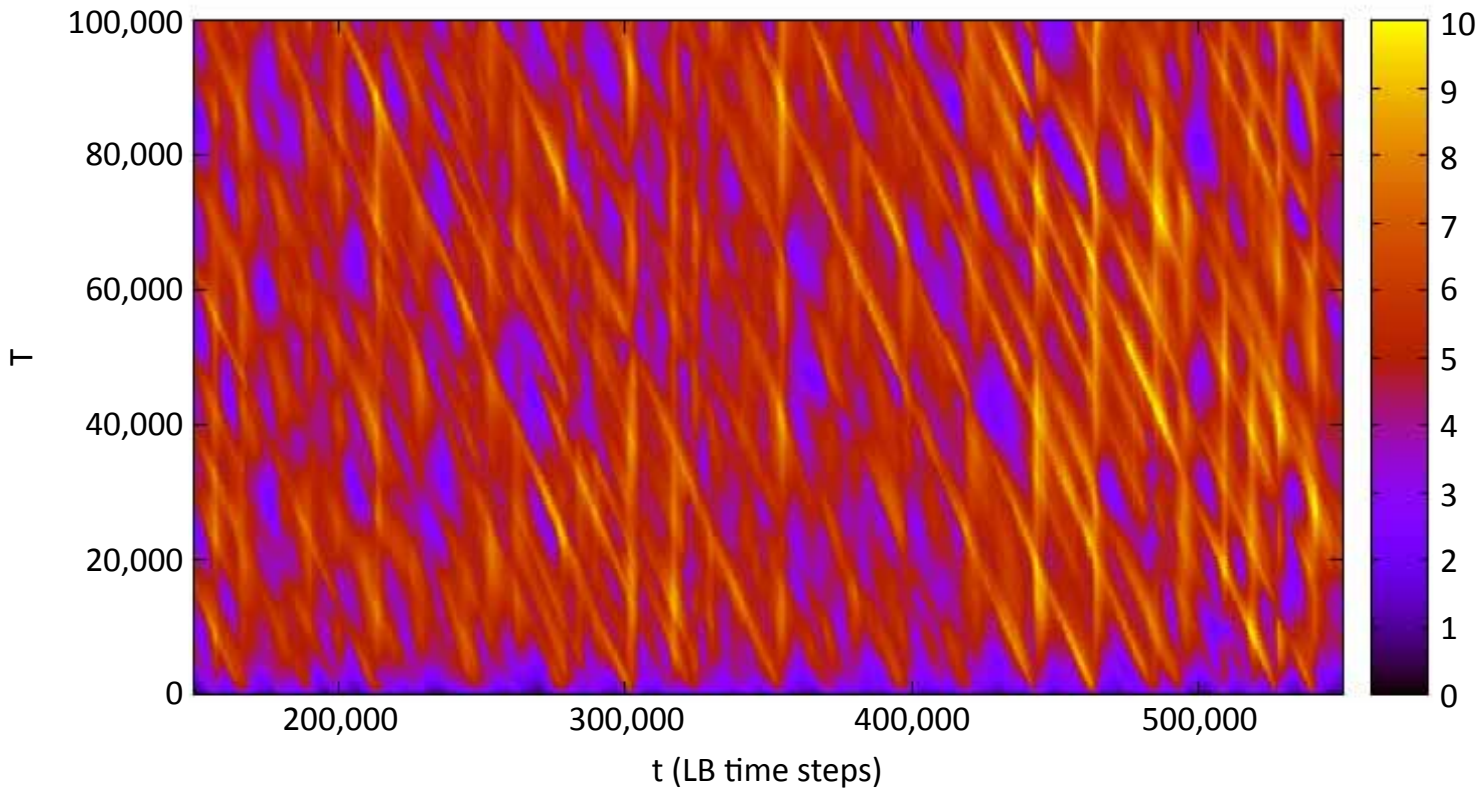
INCITE Hours Allocated on the ALCF's Blue Gene/P: 40 Million

Cerebral Blood Flow Behavior Helps Scientists Understand Cardiovascular Disease (Part III)

Large-Scale Condensed Matter and Fluid Dynamics Simulations in Three Diverse Areas

Part III: Identification of Unstable Periodic Orbits (UPOs) in the Navier-Stokes Equations

Turbulence is a paradigm problem in non-equilibrium statistical physics, with systems exhibiting large fluctuations as well as a macroscopic space-time structure. Although the Navier-Stokes equations have been known for about 150 years, a general a priori methodology for calculating statistical averages of turbulent observables, such as drag forces or heat transfer rates, still does not exist.



Part of a large comparison between 3-D time slices of a fluid in a weakly turbulent regime, with the goal of locating candidate suitable space-time orbits for the 4-D relaxation procedure. Darker regions signal less discrepancy between time slices for many different values of the period T. The system is a cubic lattice with L=64 and an ABC-force magnitude, simulated using the lattice-Boltzmann method. The Reynolds number is 371.

Scientific Approach

Researchers will locate and characterize Unstable Periodic Orbits (UPOs) in weakly turbulent hydrodynamics described by the Navier-Stokes equations. The goal is to revolutionize the statistical prediction of turbulent fluid flows using a novel four-dimensional approach that is parallel in space as well as in time.

Navier-Stokes UPOs discovered to date were found using a "shooting" algorithm, whereby the fluid equations are integrated forward in time as the inner loop of a Newton-Raphson solver whose aim is to match the initial and final conditions. Researchers intend to extend these results by using a more efficient variational approach in space-time. The goal of this proposed work is the extensive cataloging of UPOs for chaotic and turbulent systems. This project aims to provide a greater understanding of the properties of turbulent flow, including a qualitatively new way to extract them from computation. This approach fully exploits and indeed could not be implemented without the compute, memory, and disk capabilities of leadership-class resources.

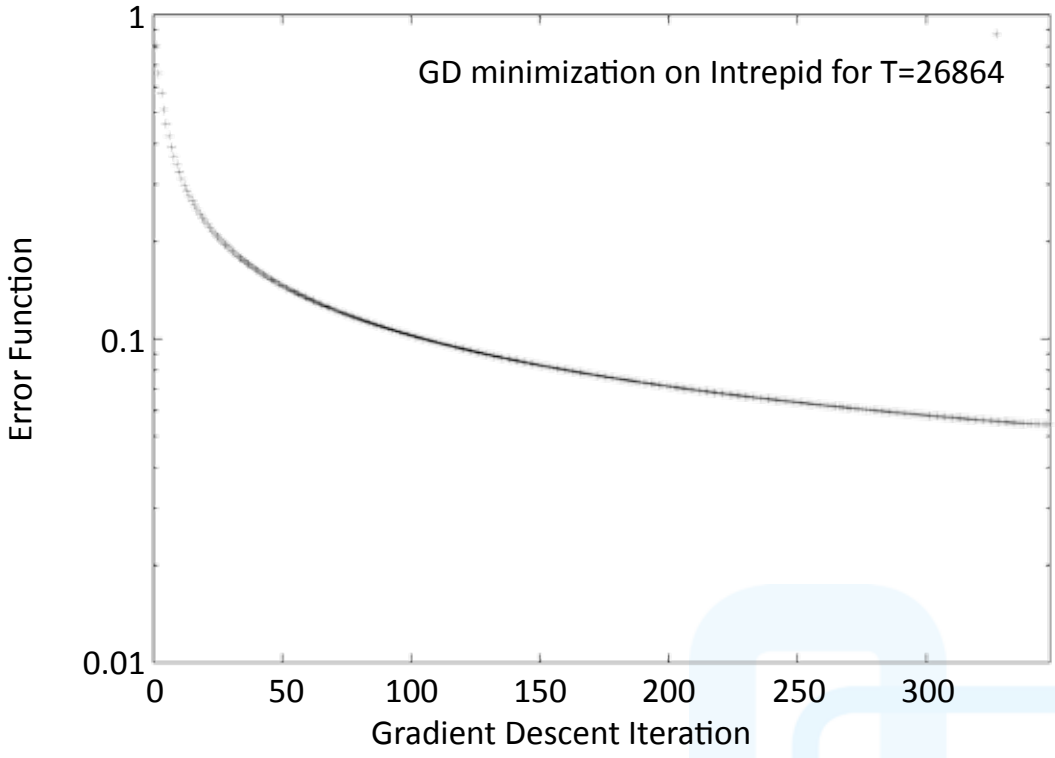
Results

Using Intrepid, researchers have successfully validated their numerical procedures. They investigated different relaxation schemes, such as gradient descent and conjugate gradients, and have optimized parameters to facilitate convergence. It is believed that these are the first trials of a space-time minimization procedure with the goal of locating UPOs on such high-dimensional dynamical systems.

Improvements to the computational model will make vessel walls elastic. The result is a far more realistic model of how blood flows through the brain.

Future Efforts

Future efforts will focus on identification of UPOs of longer periods. In particular, researchers will collect a set of the shortest-period UPOs of driven homogeneous turbulence to test the dynamical zeta function approach to extracting turbulent averages.



Results from the HYPO4D numerical relaxation procedure, showing the variation of the global error function with number of GD iterations. The system is taken from T slices of a 64 cubic lattice, with T=26864. The simulation ran on 26864 computing cores of the IBM Blue Gene/P Intrepid at the Argonne Leadership Computing Facility and took ~24 hours, including I/O and initialization. The decrease of the error function implies progressive closeness to a UPO. The RMS of the error function after 340 GD iterations is equal to 1.7504e-05.

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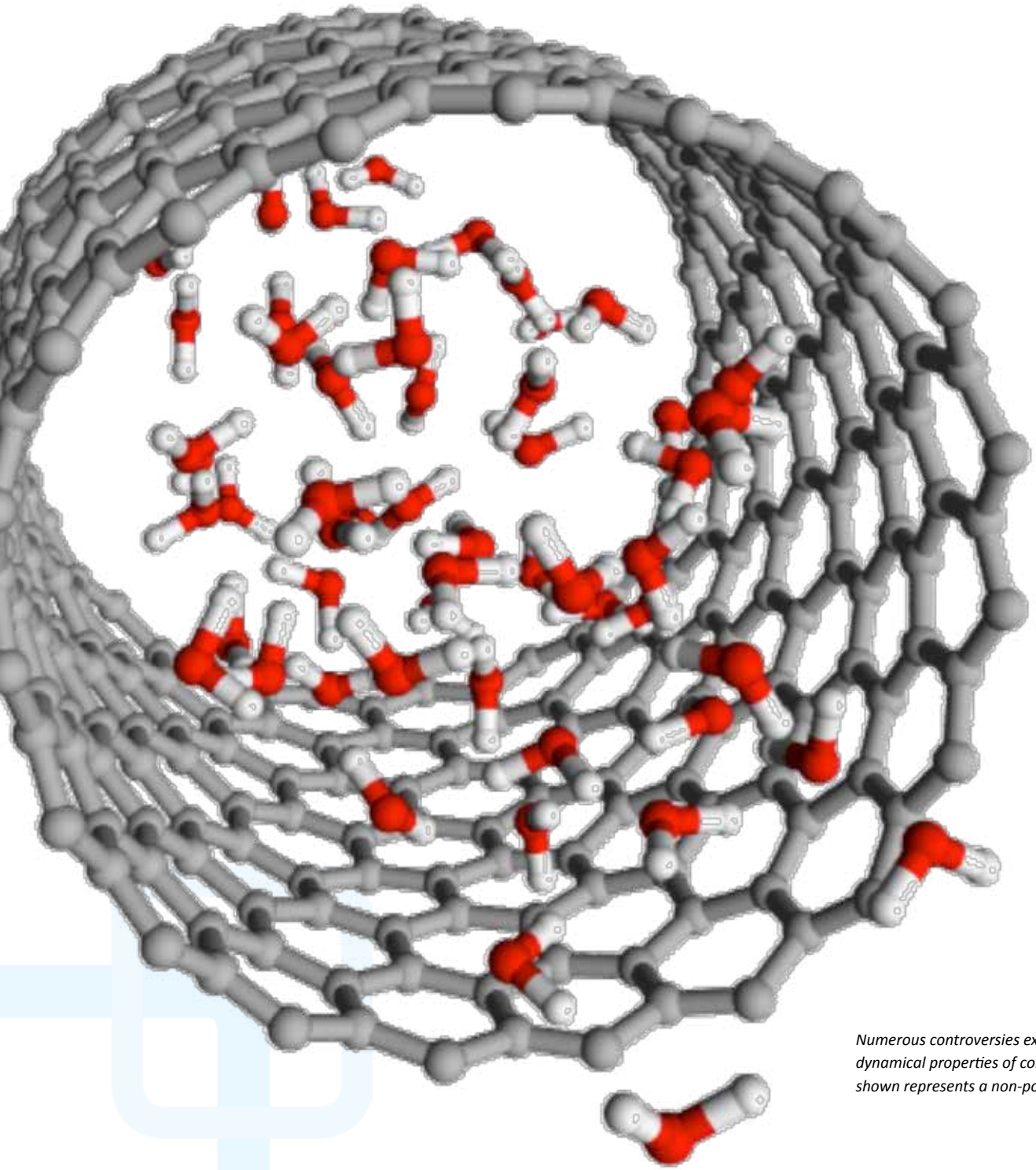
INCITE Hours Allocated on the ALCF's Blue Gene/P: 2 Million

How Are Scientists Probing the Properties of Water?

Unraveling the properties of water at organic and inorganic interfaces and under pressure is key to understanding the behavior of soft and hard materials in many natural environments and the function of biological systems. The challenging task of probing these properties is compounded when water is compressed or confined in very small spaces—within a few nanometers—as it is in the surfaces of proteins, in channels devised to transport matter at the nanoscale, or in natural rocks.



Numerous controversies exist on the structural and dynamical properties of confined water. The image shown represents a non-polar surface.

Scientific Approach

Exploiting the power of IBM Blue Gene supercomputers at the Argonne Leadership Computing Facility (ALCF) and IBM Blue Gene Watson Research Laboratory, a team of researchers is using first-principles simulations to investigate what happens at the microscopic level when water meets hydrophilic and hydrophobic surfaces and how water properties are modified at the nanoscale and under pressure. The findings can be applied to solve complex problems in both biology and materials science. The team used the Qbox code (http://eslab.ucdavis.edu/) optimized to run on high-performance platforms.

Results

To date, researchers have studied both pure water under pressure and water at interfaces with graphite, nanotubes, hydrogenated diamond surfaces, and biocompatible materials such as silicon carbide. The first-principles theory used in the team's simulations—Density Functional Theory—yields results that compare well with experiments for all the major structural properties of water, some of its electronic spectroscopic signatures, and several dynamical properties.

In addition, the key role played by electrons in determining the arrangements of water molecules at both hydrophilic and non-polar surfaces was identified. The team also computed vibrational spectra and provided predictions and interpretations of what should be seen experimentally when measuring how water molecules vibrate in contact with non-polar surfaces. Finally, the same *ab-initio* techniques recently have been applied to determine the melting line of ice under pressure; these results have been published in *Proceedings of the National Academy of Science*.

Future Efforts

Researchers will complete *ab-initio* simulations of solvated ions (alkali and halogen ions) in water confined in carbon nanotubes. They also will begin calculations of Raman spectra of water and nuclear magnetic resonance activity of water in carbon nanotubes. As for transport properties, researchers are testing viscosity calculations using classical potentials, after which they will start *ab-initio* simulations.

INCITE Contribution

"Both access to high performance computing and dedicated queues—and thus, to sustained runs—have been made possible by a DOE INCITE award. For these projects, sustained runs over several weeks were absolutely essential to obtain the results now published in premier journals, including the *Proceedings of the National Academy of Science, Physical Review Letters, and Nano Letters.*"

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

ALCF Contribution

"The use of high-performance architectures, together with access to dedicated queues at the ALCF, has made simulations possible that otherwise would not have been feasible."

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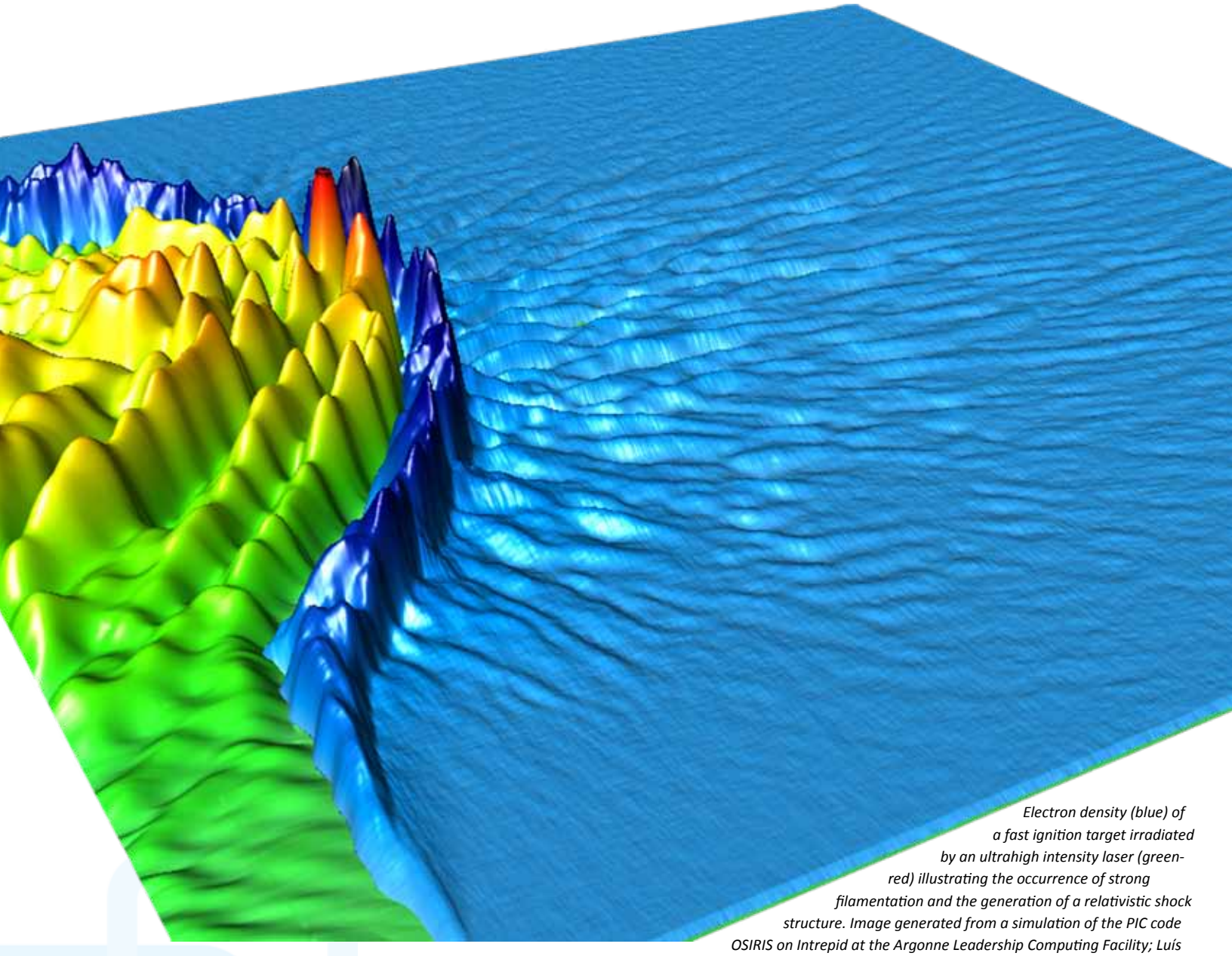
INCITE Hours Allocated on the ALCF's Blue Gene/P: 1.5 Million

Making Fusion Energy Viable

Fusion energy is regarded as a long-term energy solution that is both environmentally friendly and safe. By separating the compression phase from the ignition phase, fast ignition aims to increase fusion energy gain and the viability of inertial confinement fusion as an energy source.



Electron density (blue) of a fast ignition target irradiated by an ultrahigh intensity laser (green-red) illustrating the occurrence of strong filamentation and the generation of a relativistic shock structure. Image generated from a simulation of the PIC code OSIRIS on Intrepid at the Argonne Leadership Computing Facility; Luís Silva, IST, Portugal; Warren Mori, UCLA.

Scientific Approach

Researchers carried out first-principles-based Particle-in-Cell (PIC) simulations of the ignition phase in fast ignition (FI), using a massively parallel code, OISRIS.

Results

Using 2-D and 3-D PIC simulations, researchers were able to study the ignition phase, including laser channeling, hot electron generation, and electron transport, with unprecedented scale and detail. They found that ultra-intense lasers can be used to create a clean channel to improve the transmission of the ignition pulse and to generate electrons within the energy range suitable to ignite the target. Together, these results open up a new regime of fast ignition using ultra-intense lasers, deemed not feasible previously.

Future Efforts

By leveraging increased computer resources and improved code capability, researchers will perform more realistic simulations. A key issue is magnetic collimation in the dense plasma region, where collisions are important. In addition, they will study laser-induced relativistic shocks important to fast ignition and to astrophysics.

INCITE/ALCF Contribution

"The INCITE award, with access to Argonne Leadership Computing Facility resources, has allowed us to study critical aspects of fast ignition in great detail, and thus to better assess its overall feasibility. The award also affords us the opportunity to explore some grand-challenge problems at the frontier of high energy density physics and astrophysics."

U.S. DEPARTMENT OF ENERGY INCITE LEADERSHIP COMPUTING

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